* * * * * * * * * * * * * * * * STN Columbus * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 13:16:25 ON 09 MAY 2007

=> FILE REG

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 13:16:33 ON 09 MAY 2007
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES: 8 MAY 2007 HIGHEST RN 934461-15-1
DICTIONARY FILE UPDATES: 8 MAY 2007 HIGHEST RN 934461-15-1

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH December 2, 2006

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document. For information
on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

=>
Uploading C:\Program Files\Stnexp\Queries\10570551f.str

d 37

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:SSPTANXR1625

PASSWORD:
TERMINAL (ENTER 1, 2, 3, OR ?):2

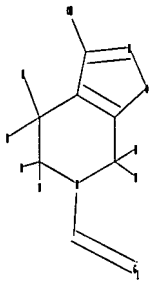
* * * * * * * * * * Welcome to STN International * * * * * * * * * *

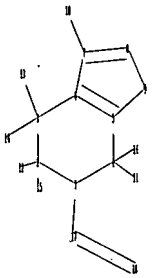
NEWS 1		Web Page for STN Seminar Schedule - N. America
NEWS 2	JAN 08	CHEMLIST enhanced with New Zealand Inventory of Chemicals
NEWS 3	JAN 16	CA/CAplus Company Name Thesaurus enhanced and reloaded
NEWS 4	JAN 16	IPC version 2007.01 thesaurus available on STN
NEWS 5	JAN 16	WPIDS/WPINDEX/WPIX enhanced with IPC 8 reclassification data
NEWS 6	JAN 22	CA/CAplus updated with revised CAS roles
NEWS 7	JAN 22	CA/CAplus enhanced with patent applications from India
NEWS 8	JAN 29	PHAR reloaded with new search and display fields
NEWS 9	JAN 29	CAS Registry Number crossover limit increased to 300,000 in multiple databases
NEWS 10	FEB 15	PATDPASPC enhanced with Drug Approval numbers
NEWS 11	FEB 15	RUSSIAPAT enhanced with pre-1994 records
NEWS 12	FEB 23	KOREAPAT enhanced with IPC 8 features and functionality
NEWS 13	FEB 26	MEDLINE reloaded with enhancements
NEWS 14	FEB 26	EMBASE enhanced with Clinical Trial Number field
NEWS 15	FEB 26	TOXCENTER enhanced with reloaded MEDLINE
NEWS 16	FEB 26	IFICDB/IFIPAT/IFIUDB reloaded with enhancements
NEWS 17	FEB 26	CAS Registry Number crossover limit increased from 10,000 to 300,000 in multiple databases
NEWS 18	MAR 15	WPIDS/WPIX enhanced with new FRAGHITSTR display format
NEWS 19	MAR 16	CASREACT coverage extended
NEWS 20	MAR 20	MARPAT now updated daily
NEWS 21	MAR 22	LWPI reloaded
NEWS 22	MAR 30	RDISCLOSURE reloaded with enhancements
NEWS 23	APR 02	JICST-EPLUS removed from database clusters and STN
NEWS 24	APR 30	GENBANK reloaded and enhanced with Genome Project ID field
NEWS 25	APR 30	CHEMCATS enhanced with 1.2 million new records
NEWS 26	APR 30	CA/CAplus enhanced with 1870-1889 U.S. patent records
NEWS 27	APR 30	INPADOC replaced by INPADOCDB on STN
NEWS 28	MAY 01	New CAS web site launched
NEWS 29	MAY 08	CA/CAplus Indian patent publication number format defined

NEWS EXPRESS NOVEMBER 10 CURRENT WINDOWS VERSION IS V8.01c, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 25 SEPTEMBER 2006.

NEWS HOURS	STN Operating Hours Plus Help Desk Availability
NEWS LOGIN	Welcome Banner and News Items
NEWS IPC8	For general information regarding STN implementation of IPC 8

Enter NEWS followed by the item number or name to see news on that specific topic.





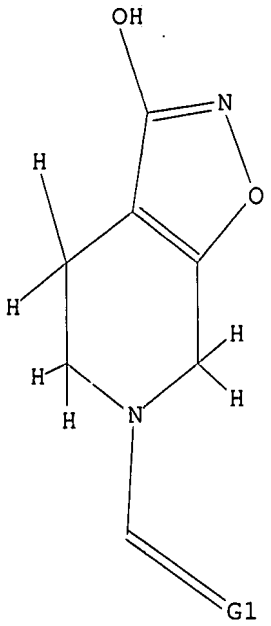
chain nodes :
10 11 12 13 14 15 16 17 18
ring nodes :
1 2 3 4 5 6 7 8 9
chain bonds :
1-17 2-12 2-15 3-13 3-14 6-11 6-16 7-10 17-18
ring bonds :
1-2 1-6 2-3 3-4 4-5 4-7 5-6 5-9 7-8 8-9
exact/norm bonds :
1-2 1-6 1-17 2-3 3-4 4-5 4-7 5-6 5-9 7-8 7-10 8-9 17-18
exact bonds :
2-12 2-15 3-13 3-14 6-11 6-16

G1:O,S,N

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS
11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS

L1 STRUCTURE UPLOADED

=> D L1
L1 HAS NO ANSWERS
L1 STR



G1 O,S,N

Structure attributes must be viewed using STN Express query preparation.

=> s l1
SAMPLE SEARCH INITIATED 13:17:20 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 2 TO ITERATE

100.0% PROCESSED 2 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 2 TO 124
PROJECTED ANSWERS: 0 TO 0

L2 0 SEA SSS SAM L1

=> s l1 full
FULL SEARCH INITIATED 13:17:25 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 55 TO ITERATE

100.0% PROCESSED 55 ITERATIONS 3 ANSWERS
SEARCH TIME: 00.00.01

L3 3 SEA SSS FUL L1

=> file caplus
COST IN U.S. DOLLARS SINCE FILE ENTRY TOTAL SESSION
FULL ESTIMATED COST 172.55 172.76

FILE 'CAPLUS' ENTERED AT 13:17:29 ON 09 MAY 2007
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

FILE COVERS 1907 - 9 May 2007 VOL 146 ISS 20
FILE LAST UPDATED: 8 May 2007 (20070508/ED)

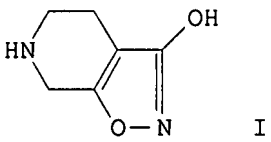
Effective October 17, 2005, revised CAS Information Use Policies apply.
They are available for your review at:

http://www.cas.org/infopolicy.html

=> s l3 full
L4 9 L3

=> d ibib abs hitstr tot

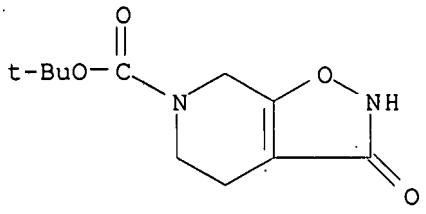
L4 ANSWER 1 OF 9 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1990:111431 CAPLUS
DOCUMENT NUMBER: 112:111431
TITLE: Enzymic synthesis of two glucuronides of the hydroxyisoxazole GABA-agonist, THIP, and the in vivo glucuronidation of THIP in rat
AUTHOR(S): Andersen, J. V.; Dalgaard, L.; Hansen, S. H.
CORPORATE SOURCE: PharmaBiote Res. Cent., R. Dan. Sch. Pharm., Copenhagen, DK-2100, Den.
SOURCE: Xenobiotica (1989), 19(12), 1399-1406
CODEN: XENOBH; ISSN: 0049-8254
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



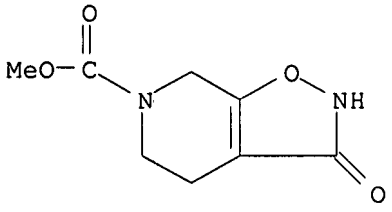
I

AB A method for the preparative enzymic synthesis of two glucuronides of THIP (3-hydroxy-4,5,6,7-tetrahydroisoxazolo[5,4-c]pyridine) (I) is described. Using FAB mass spectrometry, UV and 1H- and 13C-NMR spectroscopy, the two glucuronides were identified as N- and O-glucuronides. An HPLC method for determination of THIP and the two glucuronides in urine was developed. The glucuronidation pattern of THIP in rats was examined; THIP was excreted as THIP-O-glucuronide but not as THIP-N-glucuronide.
IT 83491-28-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and glucuronidation of)

RN 83491-28-5 CAPLUS
CN Isoxazolo[5,4-c]pyridine-6(2H)-carboxylic acid, 3,4,5,7-tetrahydro-3-oxo-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



L4 ANSWER 2 OF 9 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1985:6268 CAPLUS
DOCUMENT NUMBER: 102:6268
TITLE: Synthesis of 3-isoxazolols revisited. Diketene and β-oxo esters as starting materials
AUTHOR(S): Jacobsen, Niels; Kolind-Andersen, Hans; Christensen, Jens
CORPORATE SOURCE: Res. Dev. Dep., Cheminova Ltd., Lemvig, DK-7620, Den.
SOURCE: Canadian Journal of Chemistry (1984), 62(10), 1940-4
CODEN: CJCHAG; ISSN: 0008-4042
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 102:6268
AB 3-Isoxazolols were prepared in good yield by cyclocondensation of β-oxo esters or diketene with H2NOH, by maintaining pH .apprx.10 throughout the reaction and quenching the reaction mixture with an excess of strong mineral acid. This suppresses the formation of 5-isoxazolones, which are otherwise normally the main product of the reaction.
IT 65202-62-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, by hydroxylamine cyclocondensation with β-oxo ester)
RN 65202-62-2 CAPLUS
CN Isoxazolo[5,4-c]pyridine-6(2H)-carboxylic acid, 3,4,5,7-tetrahydro-3-oxo-, methyl ester (9CI) (CA INDEX NAME)



L4 ANSWER 3 OF 9 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1984:465548 CAPLUS
DOCUMENT NUMBER: 101:65548
TITLE: Analgesic GABA agonists. Synthesis and structure-activity studies on analogs and derivatives of muscimol and THIP
AUTHOR(S): Haefliger, Walter; Revesz, Laszlo; Maurer, Richard; Roemer, Dietmar; Buescher, Heinz Hermann
CORPORATE SOURCE: Sandoz Ltd., Basel, CH-4002, Switz.
SOURCE: European Journal of Medicinal Chemistry (1984), 19(2), 149-56
CODEN: EJMCA5; ISSN: 0009-4374
DOCUMENT TYPE: Journal
LANGUAGE: English

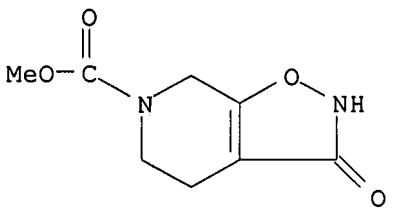
OTHER SOURCE(S): CASREACT 101:65548

AB A series of analogs. and derivs. (prodrugs) of muscimol and THIP were prepared and their GABA receptor affinity, analgesic, and GABAergic properties examined Some compds. designed as prodrugs exhibited high GABA receptor affinity indicating that nonzwitterionic mols. interact with GABA receptors. Analgesic and GABAergic activities of muscimol prodrugs were pronounced but weaker than muscimol itself. A ring opened THIP derivative was inactive whereas its carbamate derivative showed analgesic and GABAergic activity. A benzophenone-imine derivative showed strong GABA binding but no analgesic activity. Carbamate type THIP prodrugs were also active in analgesic and anticonvulsive tests but weaker than THIP itself. Ester- and alkanoyloxymethyl prodrugs were only active in the hot plate test. When the inactive 7-methyl-THIP was converted to a potential prodrug it produced high GABA-mimetic activity in both anticonvulsant and analgesic tests. In all cases, sedation was inseperable from analgesia.

IT 65202-62-2
RL: BIOL (Biological study)
(reaction with phenol sulfonyl chloride)

RN 65202-62-2 CAPLUS

CN Isoxazolo[5,4-c]pyridine-6(2H)-carboxylic acid, 3,4,5,7-tetrahydro-3-oxo-, methyl ester (9CI) (CA INDEX NAME)



L4 ANSWER 4 OF 9 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1982:582395 CAPLUS

DOCUMENT NUMBER: 97:182395

TITLE: 2-Acyl-4,5,6,7-tetrahydroisoxazolo[5,4-c]pyridin-3-ones, their use as medicines and their pharmaceutical compositions

INVENTOR(S): Perregaard, Jens Kristian

PATENT ASSIGNEE(S): Kefalas A/S, Den.

SOURCE: Fr. Demande, 18 pp.
CODEN: FRXXBL

DOCUMENT TYPE: Patent

LANGUAGE: French

FAMILY ACC. NUM. COUNT: 1

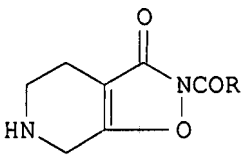
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
FR 2494691	A1	19820528	FR 1981-22328	19811127
DE 3145473	A1	19820826	DE 1981-3145473	19811116
GB 2088370	A	19820609	GB 1981-34744	19811118
GB 2088370	B	19840801		
DK 8105242	A	19820528	DK 1981-5242	19811126
JP 57118584	A	19820723	JP 1981-189409	19811127

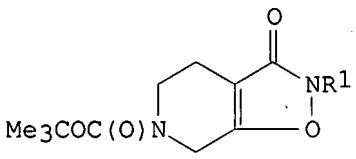
PRIORITY APPLN. INFO.: GB 1980-38140 A 19801127

OTHER SOURCE(S): CASREACT 97:182395

GI



I



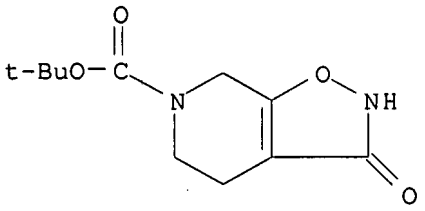
II

AB Title compds. I (R = alkyl, Ph, alkyl-, alkoxy-, or halophenyl, phenylalkyl, alkoxy, NH2, NHPh, cyclohexylamino) were prepared, and they exhibited anticonvulsant activity (formulations are also given). II (R1 = H) was heated with (PhCO)2O, and the II (R1 = COPh) obtained was treated with CF3CO2H to give I (R = Ph).

IT 83491-28-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and N-acylation of)

RN 83491-28-5 CAPLUS

CN Isoxazolo[5,4-c]pyridine-6(2H)-carboxylic acid, 3,4,5,7-tetrahydro-3-oxo-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



L4 ANSWER 5 OF 9 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1982:582394 CAPLUS

DOCUMENT NUMBER: 97:182394

TITLE: 3-Substituted 4,5,6,7-tetrahydroisoxazolo[5,4-c]pyridines and their pharmaceutical compositions

INVENTOR(S): Perregaard, Jens Kristian

PATENT ASSIGNEE(S): Kefalas A/S, Den.

SOURCE: Fr. Demande, 18 pp.
CODEN: FRXXBL

DOCUMENT TYPE: Patent

LANGUAGE: French

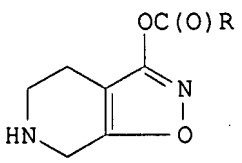
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

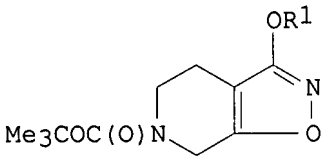
PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
FR 2494692	A1	19820528	FR 1981-22329		19811127
DE 3145474	A1	19820902	DE 1981-3145474		19811116
GB 2088371	A	19820609	GB 1981-34746		19811118
GB 2088371	B	19840718			
DK 8105241	A	19820528	DK 1981-5241		19811126
JP 57118583	A	19820723	JP 1981-189408		19811127
US 4353910	A	19821012	US 1981-325292		19811127
PRIORITY APPLN. INFO.:			GB 1980-38139	A	19801127

OTHER SOURCE(S): CASREACT 97:182394; MARPAT 97:182394

GI



I



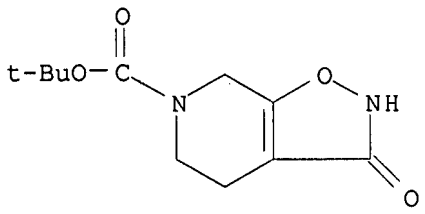
II

AB Title compds. I (R = alkyl, Ph, alkyl-, alkoxy-, or halophenyl, phenylalkyl, alkoxy, NH2, substituted amino), which were prepared, showed anticonvulsant, muscle relaxant, and analgesic activity. II (R1 = H) was treated with AcCl, and the II (R1 = Ac) product was treated with CF3CO2H to give I (R = Me).

IT 83491-28-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and O-acylation of)

RN 83491-28-5 CAPLUS

CN Isoxazolo[5,4-c]pyridine-6(2H)-carboxylic acid, 3,4,5,7-tetrahydro-3-oxo-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



L4 ANSWER 6 OF 9 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1982:562964 CAPLUS

DOCUMENT NUMBER: 97:162964

TITLE: Isoxazolo[5,4-c]pyridines which are GABA-agonists

INVENTOR(S): Krogsgaard-Larsen, Povl

PATENT ASSIGNEE(S): Lundbeck, H., og Co. A/S, Den.

SOURCE: Can., 29 pp. Division of Can. Appl. No. 305,798.
CODEN: CAXXA4

DOCUMENT TYPE: Patent

LANGUAGE: English

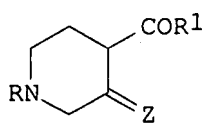
FAMILY ACC. NUM. COUNT: 3

PATENT INFORMATION:

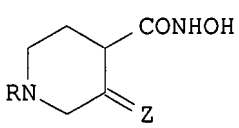
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
CA 1125288	A2	19820608	CA 1981-377128	19810507
CA 1107736	A1	19810825	CA 1978-305798	19780620
US 4301287	A	19811117	US 1979-104080	19791217
PRIORITY APPLN. INFO.:			GB 1977-25740 A	19770620
			CA 1978-305798 A3	19780620
			US 1978-917118 A3	19780619

OTHER SOURCE(S): MARPAT 97:162964

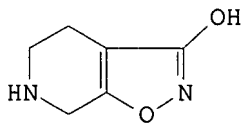
GI



I



II



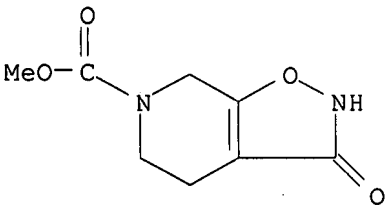
III

AB Piperidinecarboxylic acid compds. I (R = Ac, carbalkoxy, carbophenoxy, CPh3, CHO; Z = ketalized O; R1 = halo, OH, alkoxy) reacted with HONH2 to yield hydroxamic acids II. Isoxazolo[5,4-c]pyridine derivative III, which is an agonist of H2N(CH2)3CO2H, was prepared from II. I (R = CO2Me, R1 = OEt, Z = OCH2CH2O) reacted with HONH2 to give II (R = CO2Me, Z = OCH2CH2O), and the latter was treated with HCl and then with HBr-HOAc to give III.HBr.

IT 65202-62-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and hydrolysis-decarboxylation of)

RN 65202-62-2 CAPLUS

CN Isoxazolo[5,4-c]pyridine-6(2H)-carboxylic acid, 3,4,5,7-tetrahydro-3-oxo-, methyl ester (9CI) (CA INDEX NAME)



L4 ANSWER 7 OF 9 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1982:527546 CAPLUS

DOCUMENT NUMBER: 97:127546

TITLE: Deuterium labeling of the GABA agonists THIP, piperidine-4-sulfonic acid, and the GABA uptake inhibitor THPO

AUTHOR(S): Krogsgaard-Larsen, Povl; Johansen, Joergen Stage; Falch, Erik

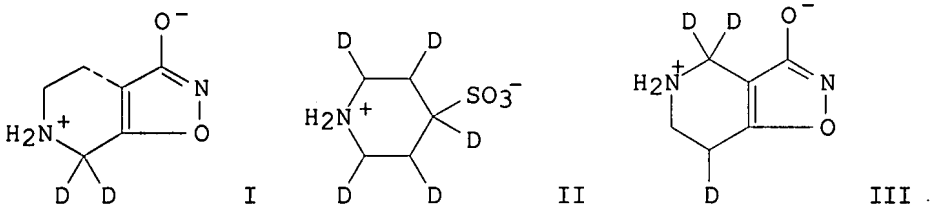
CORPORATE SOURCE: Dep. Chem. BC, R. Dan. Sch. Pharm., Copenhagen, DK-2100, Den.

SOURCE: Journal of Labelled Compounds and Radiopharmaceuticals (1982), 19(5), 689-702
CODEN: JLCRD4; ISSN: 0362-4803

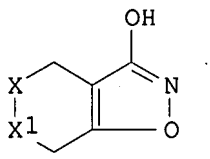
DOCUMENT TYPE: Journal

LANGUAGE: English

GI



I II III



IV

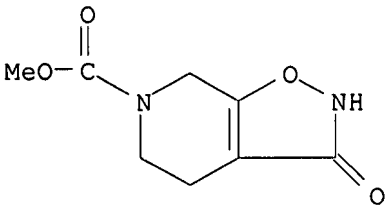
AB The D-labeled title compds. (I, II , and III, resp.) were prepared I and III were prepared from IV (X = CH2, X1 = NCO2Me; X = NCO2Me, X1 = CH2), resp., by sequential methylation, N-decarboxylation, nitrosation, H-D

exchange reaction with D2O (acid- and base-catalyzed, resp.), denitrosation, and demethylation. Pt-catalyzed deuteration of pyridine-4-sulfonic acid in D2O gave II.

IT 65202-62-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(methylation of)

RN 65202-62-2 CAPLUS

CN Isoxazolo[5,4-c]pyridine-6(2H)-carboxylic acid, 3,4,5,7-tetrahydro-3-oxo-, methyl ester (9CI) (CA INDEX NAME)

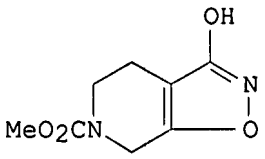


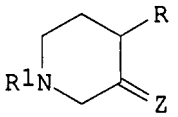
L4 ANSWER 8 OF 9 CAPLUS COPYRIGHT 2007 ACS on STN

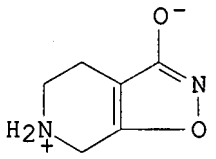
ACCESSION NUMBER: 1979:439458 CAPLUS
DOCUMENT NUMBER: 91:39458
TITLE: Methyl tetrahydrohydroxy isoxazolopyridine carboxylate
INVENTOR(S): Krogsgaard-Larsen, Povl
PATENT ASSIGNEE(S): Den.
SOURCE: Jpn. Kokai Tokkyo Koho, 13 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 54036290	A	19790316	JP 1978-74800	19780620
DK 7802702	A	19781221	DK 1978-2702	19780615
DK 7802703	A	19781221	DK 1978-2703	19780615
FI 7801954	A	19781221	FI 1978-1954	19780619
FI 64376	B	19830729		
FI 64376	C	19831110		
FI 7801955	A	19781221	FI 1978-1955	19780619
NO 7802127	A	19781221	NO 1978-2127	19780619
NO 152049	B	19850415		
NO 152449	C	19850724		
NO 7802128	A	19781221	NO 1978-2128	19780619
EP 167	A1	19790110	EP 1978-100190	19780619
R: BE, CH, DE, FR, GB, LU, NL, SE				
EP 338	A2	19790124	EP 1978-100191	19780619
EP 338	A3	19790627		
EP 338	B1	19811125		
R: BE, CH, DE, FR, GB, LU, NL, SE				
ES 470912	A1	19790201	ES 1978-470912	19780619
ES 470913	A1	19790201	ES 1978-470913	19780619
ZA 7803492	A	19790627	ZA 1978-3492	19780619
ZA 7803493	A	19790627	ZA 1978-3493	19780619
AU 7837244	A	19800103	AU 1978-37244	19780619
US 4278676	A	19810714	US 1978-917118	19780619
AU 7837298	A	19800103	AU 1978-37298	19780620
AU 521040	B2	19820311		
AT 7804486	A	19820215	AT 1978-4486	19780620
AT 368505	B	19821025		
NO 7902839	A	19781221	NO 1979-2839	19790903
US 4301287	A	19811117	US 1979-104080	19791217

EP 27279 A1 19810422 EP 1980-106497 19801023
R: BE, CH, DE, FR, GB, LU, NL, SE
EP 28017 A1 19810506 EP 1980-106498 19801023
R: BE, CH, DE, FR, GB, LU, NL, SE
PRIORITY APPLN. INFO.: GB 1977-25740 A 19770620
US 1978-917118 A3 19780619
OTHER SOURCE(S): MARPAT 91:39458
GI


I


II

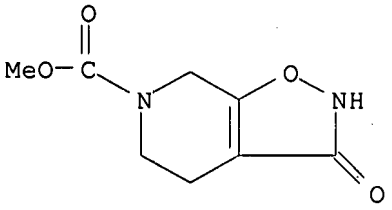

III

AB The title compound (I) was prepared Thus, (methoxycarbonyl)piperidinone II (R = CO2Et, R1 = CO2Me, Z = O) [obtained by hydrogenating II (R = CO2Et, R1 = CH2Ph, Z = O) over Pd-C, and reacting the product with ClCO2Me] was ketalized with HOCH2CH2OH to give the ethylene acetal II (R = CO2Et, R1 = CO2Me, Z = OCH2CH2O), which was treated with H2NOH.HCl to give II (R = CONHOH, R1 = CO2Me, Z = OCH2CH2O), whose cyclization in H2SO4 gave the hydroxyisoxazolopiperidinecarboxylate. Decarboxylation of I followed by treatment with HBr and then H2O-Et3N-EtOH gave zwitterion III. III was a mild tranquilizer in mice.

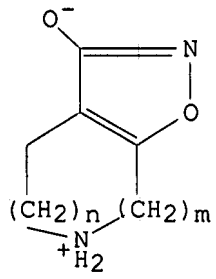
IT 65202-62-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and decarboxylation of)

RN 65202-62-2 CAPLUS

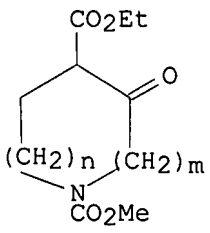
CN Isoxazolo[5,4-c]pyridine-6(2H)-carboxylic acid, 3,4,5,7-tetrahydro-3-oxo-, methyl ester (9CI) (CA INDEX NAME)



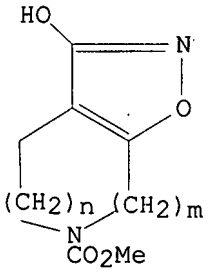
L4 ANSWER 9 OF 9 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1978:37672 CAPLUS
DOCUMENT NUMBER: 88:37672
TITLE: Muscimol analogs. II. Synthesis of some bicyclic 3-isoxazolol zwitterions
AUTHOR(S): Krogsgaard-Larsen, Povl
CORPORATE SOURCE: Dep. Chem. BC, R. Dan. Sch. Pharm., Copenhagen, Den.
SOURCE: Acta Chemica Scandinavica, Series B: Organic Chemistry and Biochemistry (1977), B31(7), 584-8
CODEN: ACBOCV; ISSN: 0302-4369
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 88:37672
GI



I



II



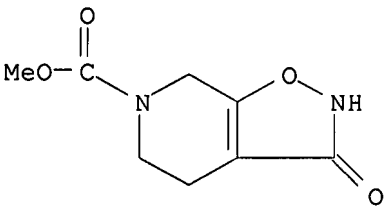
III

AB The 3-isoxazolol zwitterions 4,5,6,7-tetrahydroisoxazolo[5,4-c]pyridin-3-ol, (I, n = 1, m = 1), 5,6,7,8-tetrahydro-4H-isoxazolo[5,4-c]azepin-3-ol (I, n = 2, m = 1), and 5,6,7,8-tetrahydro-4H-isoxazolo[4,5-c]azepin-3-ol (I, n = o, m = 3) were prepared The starting materials were the cyclic β-oxoesters II. The ethylene acetals of II were treated with HONH2 followed by deacetalization and cyclization of the intermediate β-oxohydroxamic acid ethylene acetals to give the resp. 3-isoxazolol derivs. III, which were transformed into the zwitterions I. The pKA values of I were determined

IT 65202-62-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction with hydrogen bromide)

RN 65202-62-2 CAPLUS

CN Isoxazolo[5,4-c]pyridine-6(2H)-carboxylic acid, 3,4,5,7-tetrahydro-3-oxo-, methyl ester (9CI) (CA INDEX NAME)



=> d his

(FILE 'HOME' ENTERED AT 13:16:25 ON 09 MAY 2007)

FILE 'REGISTRY' ENTERED AT 13:16:33 ON 09 MAY 2007
L1 STRUCTURE UPLOADED
L2 0 S L1
L3 3 S L1 FULL

FILE 'CAPLUS' ENTERED AT 13:17:29 ON 09 MAY 2007
L4 9 S L3 FULL

=> log y

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	48.84	221.60
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-7.02	-7.02

STN INTERNATIONAL LOGOFF AT 13:19:07 ON 09 MAY 2007

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:SSPTANXR1625

PASSWORD:
TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * * * * * * Welcome to STN International * * * * * * * * * *

NEWS 1		Web Page for STN Seminar Schedule - N. America
NEWS 2	JAN 08	CHEMLIST enhanced with New Zealand Inventory of Chemicals
NEWS 3	JAN 16	CA/CAplus Company Name Thesaurus enhanced and reloaded
NEWS 4	JAN 16	IPC version 2007.01 thesaurus available on STN
NEWS 5	JAN 16	WPIDS/WPINDEX/WPIX enhanced with IPC 8 reclassification data
NEWS 6	JAN 22	CA/CAplus updated with revised CAS roles
NEWS 7	JAN 22	CA/CAplus enhanced with patent applications from India
NEWS 8	JAN 29	PHAR reloaded with new search and display fields
NEWS 9	JAN 29	CAS Registry Number crossover limit increased to 300,000 in multiple databases
NEWS 10	FEB 15	PATDPASPC enhanced with Drug Approval numbers
NEWS 11	FEB 15	RUSSIAPAT enhanced with pre-1994 records
NEWS 12	FEB 23	KOREAPAT enhanced with IPC 8 features and functionality
NEWS 13	FEB 26	MEDLINE reloaded with enhancements
NEWS 14	FEB 26	EMBASE enhanced with Clinical Trial Number field
NEWS 15	FEB 26	TOXCENTER enhanced with reloaded MEDLINE
NEWS 16	FEB 26	IFICDB/IFIPAT/IFIUDB reloaded with enhancements
NEWS 17	FEB 26	CAS Registry Number crossover limit increased from 10,000 to 300,000 in multiple databases
NEWS 18	MAR 15	WPIDS/WPIX enhanced with new FRAGHITSTR display format
NEWS 19	MAR 16	CASREACT coverage extended
NEWS 20	MAR 20	MARPAT now updated daily
NEWS 21	MAR 22	LWPI reloaded
NEWS 22	MAR 30	RDISCLOSURE reloaded with enhancements
NEWS 23	APR 02	JICST-EPLUS removed from database clusters and STN
NEWS 24	APR 30	GENBANK reloaded and enhanced with Genome Project ID field
NEWS 25	APR 30	CHEMCATS enhanced with 1.2 million new records
NEWS 26	APR 30	CA/CAplus enhanced with 1870-1889 U.S. patent records
NEWS 27	APR 30	INPADOC replaced by INPADOCDB on STN
NEWS 28	MAY 01	New CAS web site launched
NEWS 29	MAY 08	CA/CAplus Indian patent publication number format defined

NEWS EXPRESS NOVEMBER 10 CURRENT WINDOWS VERSION IS V8.01c, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 25 SEPTEMBER 2006.

NEWS HOURS	STN Operating Hours Plus Help Desk Availability
NEWS LOGIN	Welcome Banner and News Items
NEWS IPC8	For general information regarding STN implementation of IPC 8

Enter NEWS followed by the item number or name to see news on that specific topic.

* * * * * * * * * * * * * * * * STN Columbus * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 09:02:09 ON 09 MAY 2007

=> FILE CASREACT
COST IN U.S. DOLLARS

	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'CASREACT' ENTERED AT 09:02:50 ON 09 MAY 2007
USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT

FILE CONTENT:1840 - 5 May 2007 VOL 146 ISS 20

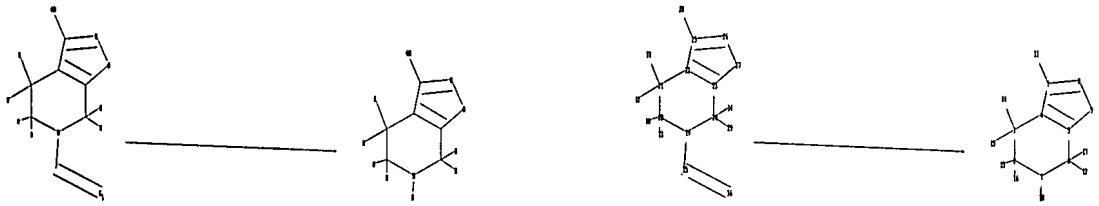
New CAS Information Use Policies, enter HELP USAGETERMS for details.

****
*
*   CASREACT now has more than 12 million reactions
*
****

Some CASREACT records are derived from the ZIC/VINITI database (1974-1999)
provided by InfoChem, INPI data prior to 1986, and Biotransformations
database compiled under the direction of Professor Dr. Klaus Kieslich.

This file contains CAS Registry Numbers for easy and accurate substance
identification.

=>
Uploading C:\Program Files\Stnexp\Queries\10570551b.str



chain nodes :
11 12 13 14 15 16 17 18 28 29 30 31 32 33 34 35 36
ring nodes :
1 2 3 4 5 6 7 8 9 19 20 21 22 23 24 25 26 27
chain bonds :
1-18 2-13 2-16 3-14 3-15 6-12 6-17 7-11 19-35 20-30 20-33 21-31 21-32
24-29 24-34 25-28 35-36
ring bonds :
1-2 1-6 2-3 3-4 4-5 4-7 5-6 5-9 7-8 8-9 19-20 19-24 20-21 21-22 22-23
22-25 23-24 23-27 25-26 26-27
exact/norm bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-11 19-20 19-24 19-35 20-21 21-22 22-23
23-24 25-26 25-28 35-36
exact bonds :
1-18 2-13 2-16 3-14 3-15 4-7 5-9 6-12 6-17 8-9 20-30 20-33 21-31 21-32
22-25 23-27 24-29 24-34 26-27
isolated ring systems :
containing 1 : 19 :

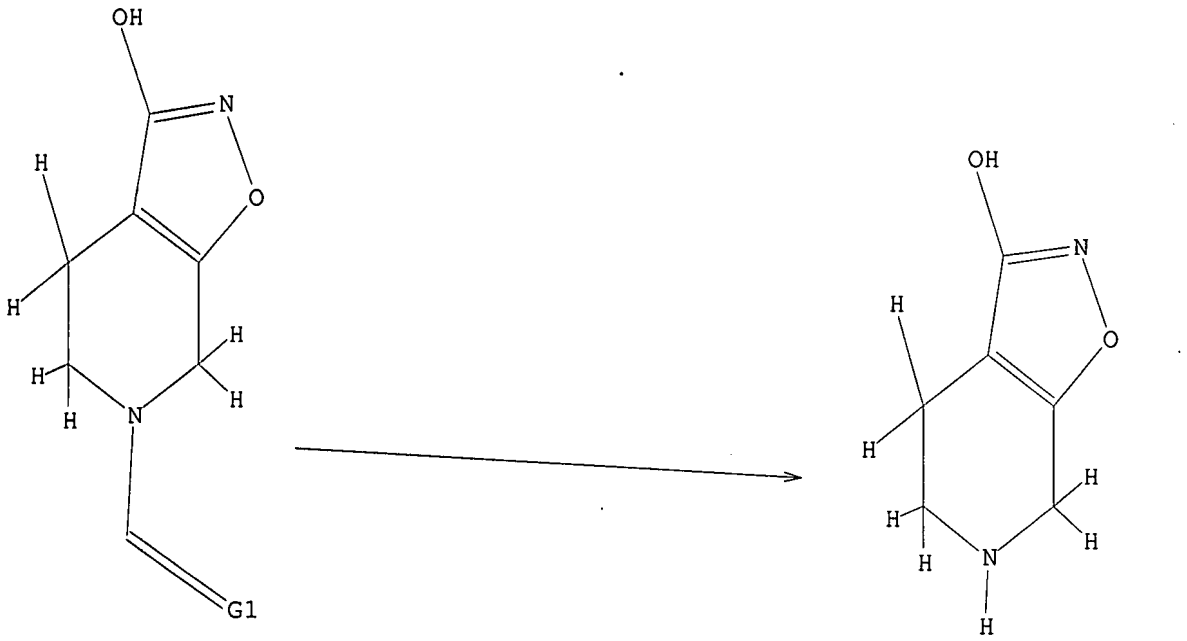
G1:O,S

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 11:CLASS
12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS 19:Atom
20:Atom 21:Atom 22:Atom 23:Atom 24:Atom 25:Atom 26:Atom 27:Atom 28:CLASS
29:CLASS 30:CLASS 31:CLASS 32:CLASS 33:CLASS 34:CLASS 35:CLASS 36:CLASS
fragments assigned product role:
containing 1
fragments assigned reactant/reagent role:

containing 19

L1 STRUCTURE UPLOADED

=> D L1
L1 HAS NO ANSWERS
L1 STR



G1 O,S

Structure attributes must be viewed using STN Express query preparation.

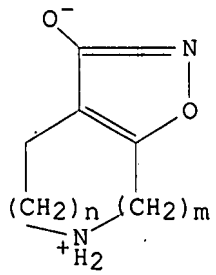
=> s l1 full
FULL SEARCH INITIATED 09:03:31 FILE 'CASREACT'
SCREENING COMPLETE - 22 REACTIONS TO VERIFY FROM 9 DOCUMENTS

100.0% DONE 22 VERIFIED 2 HIT RXNS 1 DOCS
SEARCH TIME: 00.00.01

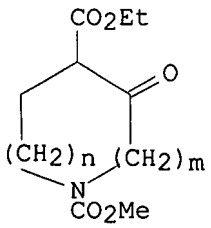
L2 1 SEA SSS FUL L1 (2 REACTIONS)

=> d ibib abs fhit

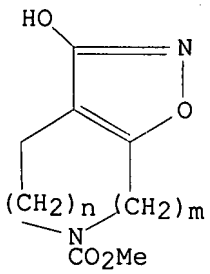
L2 ANSWER 1 OF 1 CASREACT COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 88:37672 CASREACT
TITLE: Muscimol analogs. II. Synthesis of some bicyclic 3-isoxazolol zwitterions
AUTHOR(S): Krogsgaard-Larsen, Povl
CORPORATE SOURCE: Dep. Chem. BC, R. Dan. Sch. Pharm., Copenhagen, Den.
SOURCE: Acta Chemica Scandinavica, Series B: Organic Chemistry and Biochemistry (1977), B31(7), 584-8
CODEN: ACBOCV; ISSN: 0302-4369
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I



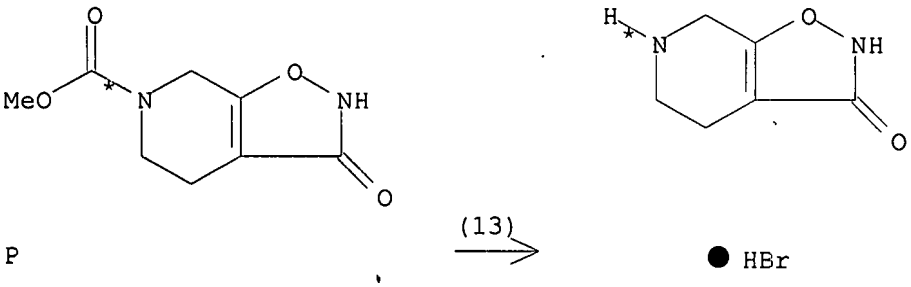
II



III

AB The 3-isoxazolol zwitterions 4,5,6,7-tetrahydroisoxazolo[5,4-c]pyridin-3-ol, (I, n = 1, m = 1), 5,6,7,8-tetrahydro-4H-isoxazolo[5,4-c]azepin-3-ol (I, n = 2, m = 1), and 5,6,7,8-tetrahydro-4H-isoxazolo[4,5-c]azepin-3-ol (I, n = o, m = 3) were prepared The starting materials were the cyclic β-oxoesters II. The ethylene acetals of II were treated with HONH2 followed by deacetalization and cyclization of the intermediate β-oxohydroxamic acid ethylene acetals to give the resp. 3-isoxazolol derivs. III, which were transformed into the zwitterions I. The pKA values of I were determined

RX(13) OF 48 ...P ===> R...



P

R

YIELD 56%

RX(13) RCT P 65202-62-2
RGT F 10035-10-6 HBr
PRO R 65202-63-3

=> FIL STNGUIDE

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	118.92	119.13

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-0.73	-0.73

FILE 'STNGUIDE' ENTERED AT 09:03:58 ON 09 MAY 2007

FILE CONTAINS CURRENT INFORMATION.
LAST RELOADED: May 4, 2007 (20070504/UP).

```
=> d his

     (FILE 'HOME' ENTERED AT 09:02:09 ON 09 MAY 2007)

     FILE 'CASREACT' ENTERED AT 09:02:50 ON 09 MAY 2007
L1              STRUCTURE UPLOADED
L2            1 S L1 FULL

     FILE 'STNGUIDE' ENTERED AT 09:03:58 ON 09 MAY 2007

=> log y
COST IN U.S. DOLLARS                                SINCE FILE     TOTAL
                                                       ENTRY   SESSION
FULL ESTIMATED COST                                     0.06    119.19

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)          SINCE FILE     TOTAL
                                                       ENTRY   SESSION
CA SUBSCRIBER PRICE                                     0.00     -0.73

STN INTERNATIONAL LOGOFF AT 09:04:14 ON 09 MAY 2007
```

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:SSPTANXR1625

PASSWORD:
TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * * * * * * Welcome to STN International * * * * * * * * * *

NEWS 1		Web Page for STN Seminar Schedule - N. America
NEWS 2	JAN 08	CHEMLIST enhanced with New Zealand Inventory of Chemicals
NEWS 3	JAN 16	CA/CAplus Company Name Thesaurus enhanced and reloaded
NEWS 4	JAN 16	IPC version 2007.01 thesaurus available on STN
NEWS 5	JAN 16	WPIDS/WPINDEX/WPIX enhanced with IPC 8 reclassification data
NEWS 6	JAN 22	CA/CAplus updated with revised CAS roles
NEWS 7	JAN 22	CA/CAplus enhanced with patent applications from India
NEWS 8	JAN 29	PHAR reloaded with new search and display fields
NEWS 9	JAN 29	CAS Registry Number crossover limit increased to 300,000 in multiple databases
NEWS 10	FEB 15	PATDPASPC enhanced with Drug Approval numbers
NEWS 11	FEB 15	RUSSIAPAT enhanced with pre-1994 records
NEWS 12	FEB 23	KOREAPAT enhanced with IPC 8 features and functionality
NEWS 13	FEB 26	MEDLINE reloaded with enhancements
NEWS 14	FEB 26	EMBASE enhanced with Clinical Trial Number field
NEWS 15	FEB 26	TOXCENTER enhanced with reloaded MEDLINE
NEWS 16	FEB 26	IFICDB/IFIPAT/IFIUDB reloaded with enhancements
NEWS 17	FEB 26	CAS Registry Number crossover limit increased from 10,000 to 300,000 in multiple databases
NEWS 18	MAR 15	WPIDS/WPIX enhanced with new FRAGHITSTR display format
NEWS 19	MAR 16	CASREACT coverage extended
NEWS 20	MAR 20	MARPAT now updated daily
NEWS 21	MAR 22	LWPI reloaded
NEWS 22	MAR 30	RDISCLOSURE reloaded with enhancements
NEWS 23	APR 02	JICST-EPLUS removed from database clusters and STN
NEWS 24	APR 30	GENBANK reloaded and enhanced with Genome Project ID field
NEWS 25	APR 30	CHEMCATS enhanced with 1.2 million new records
NEWS 26	APR 30	CA/CAplus enhanced with 1870-1889 U.S. patent records
NEWS 27	APR 30	INPADOC replaced by INPADOCDB on STN
NEWS 28	MAY 01	New CAS web site launched
NEWS 29	MAY 08	CA/CAplus Indian patent publication number format defined

NEWS EXPRESS NOVEMBER 10 CURRENT WINDOWS VERSION IS V8.01c, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 25 SEPTEMBER 2006.

NEWS HOURS	STN Operating Hours Plus Help Desk Availability
NEWS LOGIN	Welcome Banner and News Items
NEWS IPC8	For general information regarding STN implementation of IPC 8

Enter NEWS followed by the item number or name to see news on that specific topic.

* * * * * * * * * * * * * * * * STN Columbus * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 13:07:05 ON 09 MAY 2007

=> file reg
COST IN U.S. DOLLARS

	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 13:07:20 ON 09 MAY 2007
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 8 MAY 2007 HIGHEST RN 934461-15-1
DICTIONARY FILE UPDATES: 8 MAY 2007 HIGHEST RN 934461-15-1

New CAS Information Use Policies, enter HELP USAGETERMS for details.

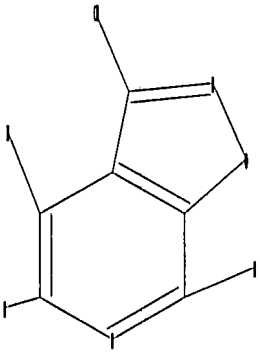
TSCA INFORMATION NOW CURRENT THROUGH December 2, 2006

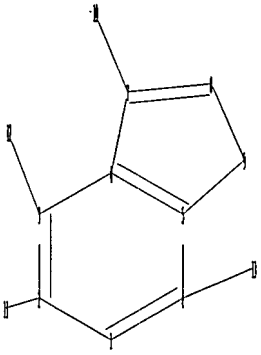
Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

=>
Uploading C:\Program Files\Stnexp\Queries\10570551d.str



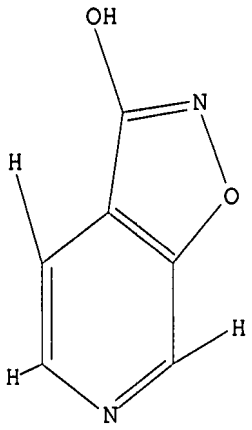


chain nodes :
10 11 12 13
ring nodes :
1 2 3 4 5 6 7 8 9
chain bonds :
2-11 3-12 6-13 7-10
ring bonds :
1-2 1-6 2-3 3-4 4-5 4-7 5-6 5-9 7-8 8-9
exact/norm bonds :
4-7 5-9 7-8 7-10 8-9
exact bonds :
2-11 3-12 6-13
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS
11:CLASS 12:CLASS 13:CLASS

L1 STRUCTURE UPLOADED

=> d l1
L1 HAS NO ANSWERS
L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l1
SAMPLE SEARCH INITIATED 13:08:10 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 1 TO ITERATE

100.0% PROCESSED 1 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 1 TO 80
PROJECTED ANSWERS: 0 TO 0

L2 0 SEA SSS SAM L1

=> s l1 full
FULL SEARCH INITIATED 13:08:14 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 26 TO ITERATE

100.0% PROCESSED 26 ITERATIONS 3 ANSWERS
SEARCH TIME: 00.00.01

L3 3 SEA SSS FUL L1

=> file caplus
COST IN U.S. DOLLARS SINCE FILE ENTRY TOTAL SESSION
FULL ESTIMATED COST 172.55 172.76

FILE 'CAPLUS' ENTERED AT 13:08:19 ON 09 MAY 2007
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

FILE COVERS 1907 - 9 May 2007 VOL 146 ISS 20
FILE LAST UPDATED: 8 May 2007 (20070508/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply.
They are available for your review at:

http://www.cas.org/infopolicy.html

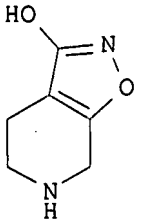
=> s l3 full
L4 1 L3

=> d ibib abs hitstr tot

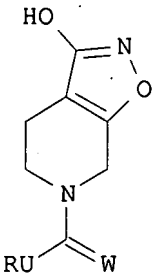
L4 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2005:238996 CAPLUS
DOCUMENT NUMBER: 142:316828
TITLE: Method for the manufacture of THIP
INVENTOR(S): Petersen, Hans; Bech Sommer, Michael; Dancer, Robert
PATENT ASSIGNEE(S): H. Lundbeck A/S, Den.
SOURCE: PCT Int. Appl., 34 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
WO 2005023820	A1	20050317	WO 2004-DK579		20040901
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW					
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG					
AU 2004270323	A1	20050317	AU 2004-270323		20040901
CA 2537840	A1	20050317	CA 2004-2537840		20040901
EP 1664060	A1	20060607	EP 2004-762799		20040901
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK, HR					
CN 1845928	A	20061011	CN 2004-80025424		20040901
BR 2004013741	A	20061024	BR 2004-13741		20040901
JP 2007504179	T	20070301	JP 2006-525046		20040901
NO 2006001424	A	20060329	NO 2006-1424		20060329
PRIORITY APPLN. INFO.:			DK 2003-1277	A	20030905
			US 2003-500422P	P	20030905
			WO 2004-DK579	W	20040901

OTHER SOURCE(S): CASREACT 142:316828; MARPAT 142:316828
GI



I

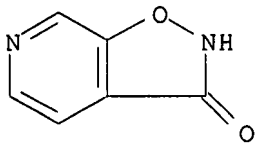


II

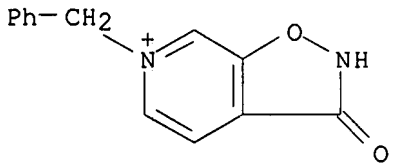
AB The present invention relates to a new method of preparing gaboxadol (THIP; I), which is useful for treating sleep disorders (no data). In particular a method of preparing THIP comprising reacting a compound II [R = alkyl, cycloalkyl, aryl, etc.; U = N, CR1 (R1 = H, R); W = O, S, NR4 (R4 = H, R)] or a salt thereof with an acid, typically a mineral acid, to obtain THIP as an acid addition salt. The present invention also relates to several intermediates. E.g., a multi-step synthesis of I.HBr, starting from Me 3-hydroxyisonicotinate, was given.

IT 847996-42-3P, Isoxazolo[5,4-c]pyridin-3(2H)-one
847996-43-4P
RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(method for the manufacture of THIP)

RN 847996-42-3 CAPLUS
CN Isoxazolo[5,4-c]pyridin-3(2H)-one (9CI) (CA INDEX NAME)



RN 847996-43-4 CAPLUS
CN Isoxazolo[5,4-c]pyridinium, 2,3-dihydro-3-oxo-6-(phenylmethyl)-, bromide (9CI) (CA INDEX NAME)



● Br^-

REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> log y

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	5.74	178.50

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-0.78	-0.78

STN INTERNATIONAL LOGOFF AT 13:08:42 ON 09 MAY 2007

d-16

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:SSPTANXR1625

PASSWORD:
TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * * * * * * Welcome to STN International * * * * * * * * * *

NEWS 1		Web Page for STN Seminar Schedule - N. America
NEWS 2	JAN 08	CHEMLIST enhanced with New Zealand Inventory of Chemicals
NEWS 3	JAN 16	CA/CAplus Company Name Thesaurus enhanced and reloaded
NEWS 4	JAN 16	IPC version 2007.01 thesaurus available on STN
NEWS 5	JAN 16	WPIDS/WPINDEX/WPIX enhanced with IPC 8 reclassification data
NEWS 6	JAN 22	CA/CAplus updated with revised CAS roles
NEWS 7	JAN 22	CA/CAplus enhanced with patent applications from India
NEWS 8	JAN 29	PHAR reloaded with new search and display fields
NEWS 9	JAN 29	CAS Registry Number crossover limit increased to 300,000 in multiple databases
NEWS 10	FEB 15	PATDPASPC enhanced with Drug Approval numbers
NEWS 11	FEB 15	RUSSIAPAT enhanced with pre-1994 records
NEWS 12	FEB 23	KOREAPAT enhanced with IPC 8 features and functionality
NEWS 13	FEB 26	MEDLINE reloaded with enhancements
NEWS 14	FEB 26	EMBASE enhanced with Clinical Trial Number field
NEWS 15	FEB 26	TOXCENTER enhanced with reloaded MEDLINE
NEWS 16	FEB 26	IFICDB/IFIPAT/IFIUDB reloaded with enhancements
NEWS 17	FEB 26	CAS Registry Number crossover limit increased from 10,000 to 300,000 in multiple databases
NEWS 18	MAR 15	WPIDS/WPIX enhanced with new FRAGHITSTR display format
NEWS 19	MAR 16	CASREACT coverage extended
NEWS 20	MAR 20	MARPAT now updated daily
NEWS 21	MAR 22	LWPI reloaded
NEWS 22	MAR 30	RDISCLOSURE reloaded with enhancements
NEWS 23	APR 02	JICST-EPLUS removed from database clusters and STN
NEWS 24	APR 30	GENBANK reloaded and enhanced with Genome Project ID field
NEWS 25	APR 30	CHEMCATS enhanced with 1.2 million new records
NEWS 26	APR 30	CA/CAplus enhanced with 1870-1889 U.S. patent records
NEWS 27	APR 30	INPADOC replaced by INPADOCDB on STN
NEWS 28	MAY 01	New CAS web site launched
NEWS 29	MAY 08	CA/CAplus Indian patent publication number format defined

NEWS EXPRESS NOVEMBER 10 CURRENT WINDOWS VERSION IS V8.01c, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 25 SEPTEMBER 2006.

NEWS HOURS	STN Operating Hours Plus Help Desk Availability
NEWS LOGIN	Welcome Banner and News Items
NEWS IPC8	For general information regarding STN implementation of IPC 8

Enter NEWS followed by the item number or name to see news on that specific topic.

* * * * * * * * * * * * * * * * STN Columbus * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 13:02:27 ON 09 MAY 2007

=> file reg
COST IN U.S. DOLLARS

	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 13:02:36 ON 09 MAY 2007
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES: 8 MAY 2007 HIGHEST RN 934461-15-1
DICTIONARY FILE UPDATES: 8 MAY 2007 HIGHEST RN 934461-15-1

New CAS Information Use Policies, enter HELP USAGETERMS for details.

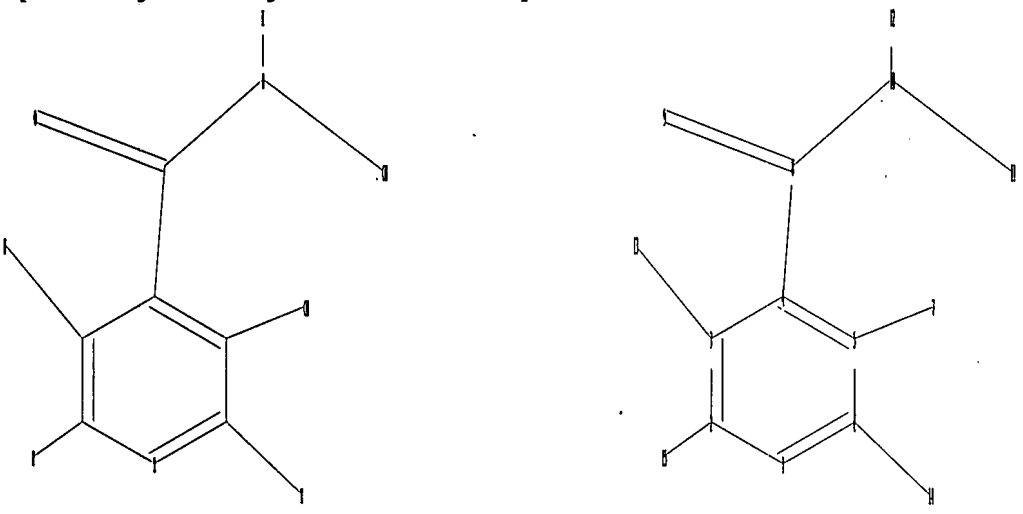
TSCA INFORMATION NOW CURRENT THROUGH December 2, 2006

Please note that search-term pricing does apply when
conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document. For information
on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

=>
Uploading C:\Program Files\Stnexp\Queries\10570551e.str



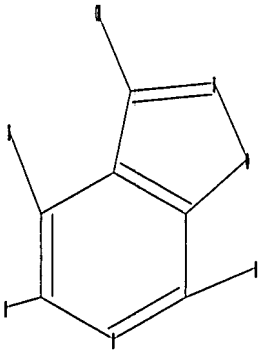
chain nodes :
7 8 9 10 11 12 13 14 15
ring nodes :
1 2 3 4 5 6
chain bonds :
2-15 3-13 4-8 5-7 6-14 8-9 8-10 10-11 10-12
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6
exact/norm bonds :
5-7 8-9 8-10 10-11

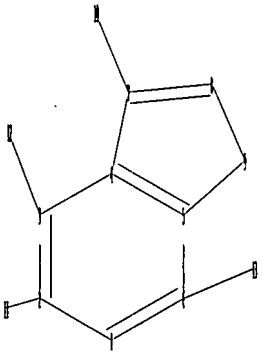
exact bonds :
2-15 3-13 4-8 6-14 10-12
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6
isolated ring systems :
containing 1 :

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS
 11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS

L1   STRUCTURE UPLOADED

=>
Uploading C:\Program Files\Stnexp\Queries\10570551d.str



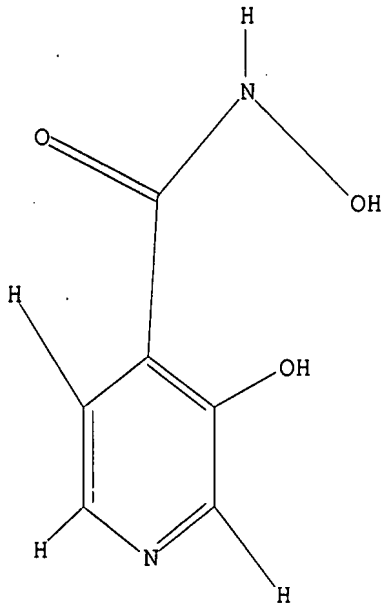


chain nodes :
10 11 12 13
ring nodes :
1 2 3 4 5 6 7 8 9
chain bonds :
2-11 3-12 6-13 7-10
ring bonds :
1-2 1-6 2-3 3-4 4-5 4-7 5-6 5-9 7-8 8-9
exact/norm bonds :
4-7 5-9 7-8 7-10 8-9
exact bonds :
2-11 3-12 6-13
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS
11:CLASS 12:CLASS 13:CLASS

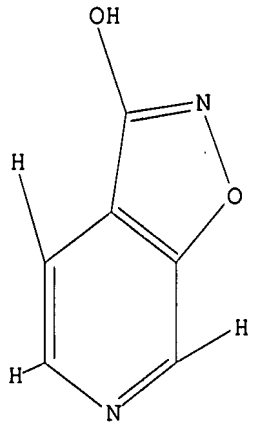
L2   STRUCTURE UPLOADED

=> d l1
L1 HAS NO ANSWERS
L1   STR



Structure attributes must be viewed using STN Express query preparation.

```
=> d l2
L2 HAS NO ANSWERS
L2                STR
```



Structure attributes must be viewed using STN Express query preparation.

```
=> s l1 full
FULL SEARCH INITIATED 13:03:49 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -      277 TO ITERATE

100.0% PROCESSED      277 ITERATIONS                                 1 ANSWERS
SEARCH TIME: 00.00.01

L3            1 SEA SSS FUL L1

=> s l2 full
FULL SEARCH INITIATED 13:04:04 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -       26 TO ITERATE
```

```
100.0% PROCESSED       26 ITERATIONS                          3 ANSWERS
SEARCH TIME: 00.00.01

L4             3 SEA SSS FUL L2

=> s l3 and l4 full
L5             0 L3 AND L4

=> log y
COST IN U.S. DOLLARS                          SINCE FILE      TOTAL
                                                   ENTRY    SESSION
FULL ESTIMATED COST                               344.65     344.86

STN INTERNATIONAL LOGOFF AT 13:04:16 ON 09 MAY 2007
```

Connecting via Winsock to STN

d 1

Welcome to STN International! Enter x:x

LOGINID:SSPTANXR1625

PASSWORD:
TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * * * * * * Welcome to STN International * * * * * * * * * *

NEWS 1		Web Page for STN Seminar Schedule - N. America
NEWS 2	JAN 08	CHEMLIST enhanced with New Zealand Inventory of Chemicals
NEWS 3	JAN 16	CA/CAplus Company Name Thesaurus enhanced and reloaded
NEWS 4	JAN 16	IPC version 2007.01 thesaurus available on STN
NEWS 5	JAN 16	WPIDS/WPINDEX/WPIX enhanced with IPC 8 reclassification data
NEWS 6	JAN 22	CA/CAplus updated with revised CAS roles
NEWS 7	JAN 22	CA/CAplus enhanced with patent applications from India
NEWS 8	JAN 29	PHAR reloaded with new search and display fields
NEWS 9	JAN 29	CAS Registry Number crossover limit increased to 300,000 in multiple databases
NEWS 10	FEB 15	PATDPASPC enhanced with Drug Approval numbers
NEWS 11	FEB 15	RUSSIAPAT enhanced with pre-1994 records
NEWS 12	FEB 23	KOREAPAT enhanced with IPC 8 features and functionality
NEWS 13	FEB 26	MEDLINE reloaded with enhancements
NEWS 14	FEB 26	EMBASE enhanced with Clinical Trial Number field
NEWS 15	FEB 26	TOXCENTER enhanced with reloaded MEDLINE
NEWS 16	FEB 26	IFICDB/IFIPAT/IFIUDB reloaded with enhancements
NEWS 17	FEB 26	CAS Registry Number crossover limit increased from 10,000 to 300,000 in multiple databases
NEWS 18	MAR 15	WPIDS/WPIX enhanced with new FRAGHITSTR display format
NEWS 19	MAR 16	CASREACT coverage extended
NEWS 20	MAR 20	MARPAT now updated daily
NEWS 21	MAR 22	LWPI reloaded
NEWS 22	MAR 30	RDISCLOSURE reloaded with enhancements
NEWS 23	APR 02	JICST-EPLUS removed from database clusters and STN
NEWS 24	APR 30	GENBANK reloaded and enhanced with Genome Project ID field
NEWS 25	APR 30	CHEMCATS enhanced with 1.2 million new records
NEWS 26	APR 30	CA/CAplus enhanced with 1870-1889 U.S. patent records
NEWS 27	APR 30	INPADOC replaced by INPADOCDB on STN
NEWS 28	MAY 01	New CAS web site launched
NEWS 29	MAY 08	CA/CAplus Indian patent publication number format defined

NEWS EXPRESS NOVEMBER 10 CURRENT WINDOWS VERSION IS V8.01c, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 25 SEPTEMBER 2006.

NEWS HOURS	STN Operating Hours Plus Help Desk Availability
NEWS LOGIN	Welcome Banner and News Items
NEWS IPC8	For general information regarding STN implementation of IPC 8

Enter NEWS followed by the item number or name to see news on that specific topic.

* * * * * * * * * * * * * * * * STN Columbus * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 12:52:51 ON 09 MAY 2007

=> file reg
COST IN U.S. DOLLARS

	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 12:53:03 ON 09 MAY 2007
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES: 8 MAY 2007 HIGHEST RN 934461-15-1
DICTIONARY FILE UPDATES: 8 MAY 2007 HIGHEST RN 934461-15-1

New CAS Information Use Policies, enter HELP USAGETERMS for details.

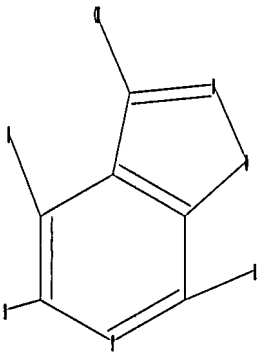
TSCA INFORMATION NOW CURRENT THROUGH December 2, 2006

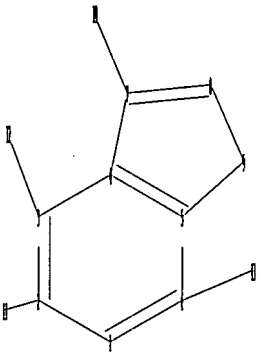
Please note that search-term pricing does apply when
conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document. For information
on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

=>
Uploading C:\Program Files\Stnexp\Queries\10570551d.str



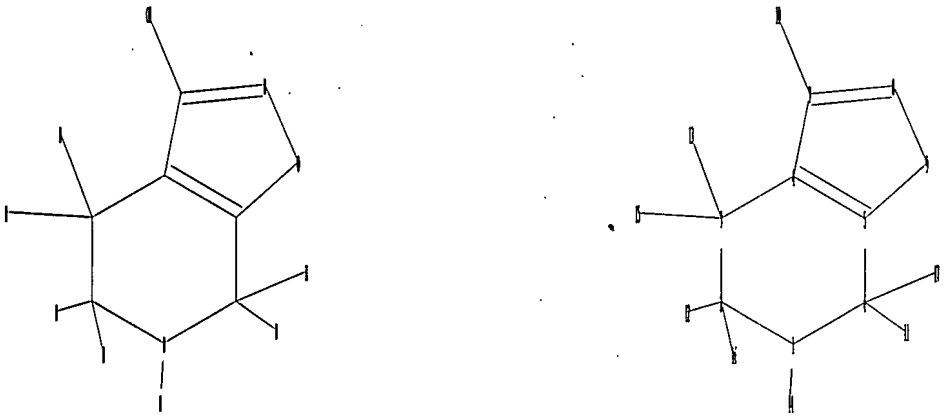


chain nodes :
10 11 12 13
ring nodes :
1 2 3 4 5 6 7 8 9
chain bonds :
2-11 3-12 6-13 7-10
ring bonds :
1-2 1-6 2-3 3-4 4-5 4-7 5-6 5-9 7-8 8-9
exact/norm bonds :
4-7 5-9 7-8 7-10 8-9
exact bonds :
2-11 3-12 6-13
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS
11:CLASS 12:CLASS 13:CLASS

L1 STRUCTURE UPLOADED

=>
Uploading C:\Program Files\Stnexp\Queries\10570551C.str

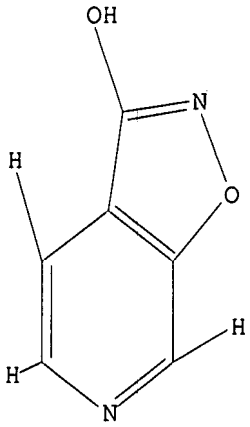


chain nodes :
10 11 12 13 14 15 16 17
ring nodes :
1 2 3 4 5 6 7 8 9
chain bonds :
1-14 2-12 2-16 3-13 3-15 6-11 6-17 7-10
ring bonds :
1-2 1-6 2-3 3-4 4-5 4-7 5-6 5-9 7-8 8-9
exact/norm bonds :
1-2 1-6 2-3 3-4 4-5 4-7 5-6 5-9 7-8 7-10 8-9
exact bonds :
1-14 2-12 2-16 3-13 3-15 6-11 6-17

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS
11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS

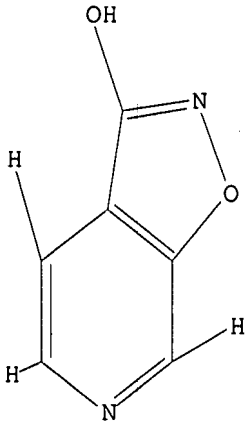
L2 STRUCTURE UPLOADED

=> d l1
L1 HAS NO ANSWERS
L1 STR



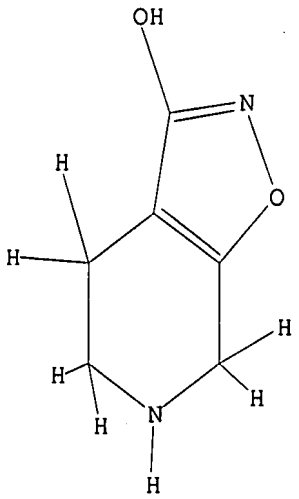
Structure attributes must be viewed using STN Express query preparation.

=> d l1
L1 HAS NO ANSWERS
L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> d l2
L2 HAS NO ANSWERS
L2 STR



Structure attributes must be viewed using STN Express query preparation.

```
=> s l1 full
FULL SEARCH INITIATED 12:54:07 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -       26 TO ITERATE

100.0% PROCESSED       26 ITERATIONS                                3 ANSWERS
SEARCH TIME: 00.00.01

L3             3 SEA SSS FUL L1

=> s l2 ful
FULL SEARCH INITIATED 12:54:11 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -      261 TO ITERATE

100.0% PROCESSED      261 ITERATIONS                               36 ANSWERS
SEARCH TIME: 00.00.01

L4            36 SEA SSS FUL L2

=> s l3 and l4
L5             0 L3 AND L4

=> log y
COST IN U.S. DOLLARS                          SINCE FILE      TOTAL
                                                 ENTRY    SESSION
FULL ESTIMATED COST                             344.20     344.41

STN INTERNATIONAL LOGOFF AT 12:54:28 ON 09 MAY 2007
```

Q: 1

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:SSPTANXR1625

PASSWORD:
TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * * * * * * Welcome to STN International * * * * * * * * * *

NEWS 1		Web Page for STN Seminar Schedule - N. America
NEWS 2	JAN 08	CHEMLIST enhanced with New Zealand Inventory of Chemicals
NEWS 3	JAN 16	CA/CAplus Company Name Thesaurus enhanced and reloaded
NEWS 4	JAN 16	IPC version 2007.01 thesaurus available on STN
NEWS 5	JAN 16	WPIDS/WPINDEX/WPIX enhanced with IPC 8 reclassification data
NEWS 6	JAN 22	CA/CAplus updated with revised CAS roles
NEWS 7	JAN 22	CA/CAplus enhanced with patent applications from India
NEWS 8	JAN 29	PHAR reloaded with new search and display fields
NEWS 9	JAN 29	CAS Registry Number crossover limit increased to 300,000 in multiple databases
NEWS 10	FEB 15	PATDPASPC enhanced with Drug Approval numbers
NEWS 11	FEB 15	RUSSIAPAT enhanced with pre-1994 records
NEWS 12	FEB 23	KOREAPAT enhanced with IPC 8 features and functionality
NEWS 13	FEB 26	MEDLINE reloaded with enhancements
NEWS 14	FEB 26	EMBASE enhanced with Clinical Trial Number field
NEWS 15	FEB 26	TOXCENTER enhanced with reloaded MEDLINE
NEWS 16	FEB 26	IFICDB/IFIPAT/IFIUDB reloaded with enhancements
NEWS 17	FEB 26	CAS Registry Number crossover limit increased from 10,000 to 300,000 in multiple databases
NEWS 18	MAR 15	WPIDS/WPIX enhanced with new FRAGHITSTR display format
NEWS 19	MAR 16	CASREACT coverage extended
NEWS 20	MAR 20	MARPAT now updated daily
NEWS 21	MAR 22	LWPI reloaded
NEWS 22	MAR 30	RDISCLOSURE reloaded with enhancements
NEWS 23	APR 02	JICST-EPLUS removed from database clusters and STN
NEWS 24	APR 30	GENBANK reloaded and enhanced with Genome Project ID field
NEWS 25	APR 30	CHEMCATS enhanced with 1.2 million new records
NEWS 26	APR 30	CA/CAplus enhanced with 1870-1889 U.S. patent records
NEWS 27	APR 30	INPADOC replaced by INPADOCDB on STN
NEWS 28	MAY 01	New CAS web site launched
NEWS 29	MAY 08	CA/CAplus Indian patent publication number format defined

NEWS EXPRESS NOVEMBER 10 CURRENT WINDOWS VERSION IS V8.01c, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 25 SEPTEMBER 2006.

NEWS HOURS	STN Operating Hours Plus Help Desk Availability
NEWS LOGIN	Welcome Banner and News Items
NEWS IPC8	For general information regarding STN implementation of IPC 8

Enter NEWS followed by the item number or name to see news on that specific topic.

* * * * * * * * * * * * * * * * STN Columbus * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 12:37:09 ON 09 MAY 2007

=>
Uploading
THIS COMMAND NOT AVAILABLE IN THE CURRENT FILE
Do you want to switch to the Registry File?
Choice (Y/n):
Switching to the Registry File...
Some commands only work in certain files. For example, the EXPAND command can only be used to look at the index in a file which has an index. Enter "HELP COMMANDS" at an arrow prompt (=>) for a list of commands which can be used in this file.

=> FILE REGISTRY

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.42	0.42

FILE 'REGISTRY' ENTERED AT 12:38:04 ON 09 MAY 2007
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 8 MAY 2007 HIGHEST RN 934461-15-1
DICTIONARY FILE UPDATES: 8 MAY 2007 HIGHEST RN 934461-15-1

New CAS Information Use Policies, enter HELP USAGETERMS for details.

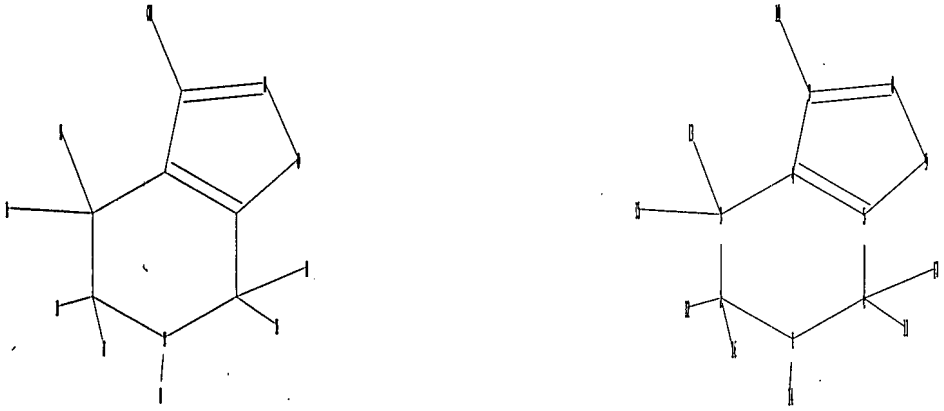
TSCA INFORMATION NOW CURRENT THROUGH December 2, 2006

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

=>
Uploading C:\Program Files\Stnexp\Queries\10570551C.str



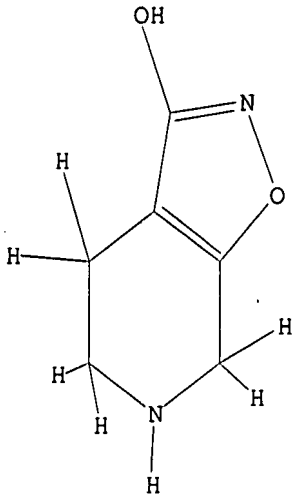
chain nodes :

```
10  11  12  13  14  15  16  17
ring nodes :
1  2  3  4  5  6  7  8  9
chain bonds :
1-14  2-12  2-16  3-13  3-15  6-11  6-17  7-10
ring bonds :
1-2  1-6  2-3  3-4  4-5  4-7  5-6  5-9  7-8  8-9
exact/norm bonds :
1-2  1-6  2-3  3-4  4-5  4-7  5-6  5-9  7-8  7-10  8-9
exact bonds :
1-14  2-12  2-16  3-13  3-15  6-11  6-17

Match level :
1:Atom  2:Atom  3:Atom  4:Atom  5:Atom  6:Atom  7:Atom  8:Atom  9:Atom  10:CLASS
11:CLASS  12:CLASS  13:CLASS  14:CLASS  15:CLASS  16:CLASS  17:CLASS


L1      STRUCTURE UPLOADED

=> D L1
L1 HAS NO ANSWERS
L1              STR
```




```
Structure attributes must be viewed using STN Express query preparation.


=> s l1 full
FULL SEARCH INITIATED 12:41:39 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -      261 TO ITERATE

100.0% PROCESSED      261 ITERATIONS                              36 ANSWERS
SEARCH TIME: 00.00.01

L2          36 SEA SSS FUL L1

=> file caplus
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                       ENTRY    SESSION
FULL ESTIMATED COST                                   174.35     174.77

FILE 'CAPLUS' ENTERED AT 12:41:50 ON 09 MAY 2007
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
```

PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

FILE COVERS 1907 - 9 May 2007 VOL 146 ISS 20
FILE LAST UPDATED: 8 May 2007 (20070508/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply.
They are available for your review at:

http://www.cas.org/infopolicy.html

```
=> s l2/prep full
           481 L2
       4400083 PREP/RL
L3          13 L2/PREP
                 (L2 (L) PREP/RL)

=> s l3 and nucleo?
        742508 NUCLEO?
L4           0 L3 AND NUCLEO?

=> d ibib abs hitstr l3 tot
```

L3 ANSWER 1 OF 13 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2006:1177390 CAPLUS
DOCUMENT NUMBER: 145:495605
TITLE: Acid and base salt forms of gaboxadol
INVENTOR(S): Crocker, Louis S.; Murry, Jerry A.; Nagapudi, Karthik; Rubin, Kara Beth
PATENT ASSIGNEE(S): Merck & Co., Inc., USA
SOURCE: PCT Int. Appl., 20pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2006118897	A1	20061109	WO 2006-US15789	20060425

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

PRIORITY APPLN. INFO.: US 2005-676332P P 20050429

AB The present invention is directed to novel acid salt forms and base salt

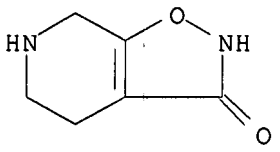
forms of the compound gaboxadol (4,5,6,7-tetrahydroisoxazolo[5,4-c]pyridin-3-ol) and hydrates, solvates and polymorphic forms thereof. The invention is further concerned with pharmaceutical compns. containing the salt forms as an active ingredient, methods for treatment of disorders susceptible to amelioration by GABAA receptor agonism with the salt forms, and processes for the preparation of the salt forms.

IT 914291-56-8P 914291-57-9P 914291-58-0P
914291-59-1P 914291-60-4P 914291-62-6P
914291-64-8P 914291-66-0P 914291-67-1P
914291-68-2P 914291-69-3P 914291-71-7P
914291-72-8P 914291-73-9P
RL: PEP (Physical, engineering or chemical process); PYP (Physical process); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); PROC (Process); USES (Uses)
(acid and base salt forms of gaboxadol)

RN 914291-56-8 CAPLUS
CN Isoxazolo[5,4-c]pyridin-3(2H)-one, 4,5,6,7-tetrahydro-, monoacetate (9CI) (CA INDEX NAME)

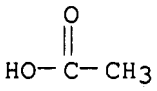
CM 1

CRN 64603-91-4
CMF C6 H8 N2 O2



CM 2

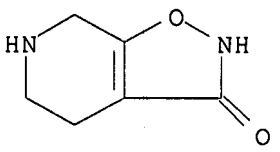
CRN 64-19-7
CMF C2 H4 O2



RN 914291-57-9 CAPLUS
CN Isoxazolo[5,4-c]pyridin-3(2H)-one, 4,5,6,7-tetrahydro-, 2-hydroxy-1,2,3-propanetricarboxylate (3:1) (9CI) (CA INDEX NAME)

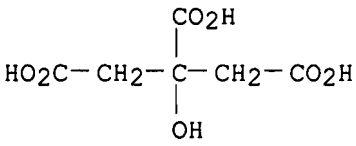
CM 1

CRN 64603-91-4
CMF C6 H8 N2 O2



CM 2

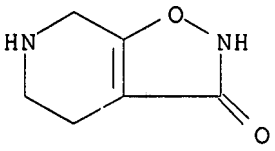
CRN 77-92-9
CMF C6 H8 O7



RN 914291-58-0 CAPLUS
CN Isoxazolo[5,4-c]pyridin-3(2H)-one, 4,5,6,7-tetrahydro-, (2E)-2-butenedioate (2:1) (9CI) (CA INDEX NAME)

CM 1

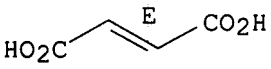
CRN 64603-91-4
CMF C6 H8 N2 O2



CM 2

CRN 110-17-8
CMF C4 H4 O4

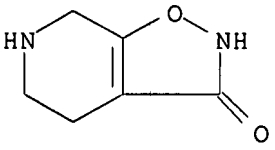
Double bond geometry as shown.



RN 914291-59-1 CAPLUS
CN Isoxazolo[5,4-c]pyridin-3(2H)-one, 4,5,6,7-tetrahydro-, phosphate (3:1) (9CI) (CA INDEX NAME)

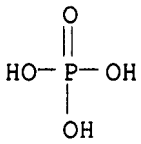
CM 1

CRN 64603-91-4
CMF C6 H8 N2 O2



CM 2

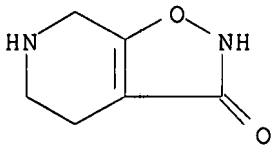
CRN 7664-38-2
CMF H3 O4 P



RN 914291-60-4 CAPLUS
CN Isoxazolo[5,4-c]pyridin-3(2H)-one, 4,5,6,7-tetrahydro-, (2R,3R)-2,3-dihydroxybutanedioate (2:1) (9CI) (CA INDEX NAME)

CM 1

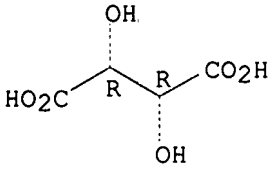
CRN 64603-91-4
CMF C6 H8 N2 O2



CM 2

CRN 87-69-4
CMF C4 H6 O6

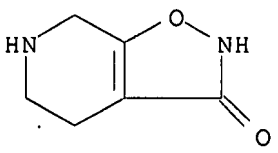
Absolute stereochemistry.



RN 914291-62-6 CAPLUS
CN Butanedioic acid, compd. with 4,5,6,7-tetrahydroisoxazolo[5,4-c]pyridin-3(2H)-one (1:2) (9CI) (CA INDEX NAME)

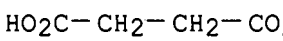
CM 1

CRN 64603-91-4
CMF C6 H8 N2 O2



CM 2

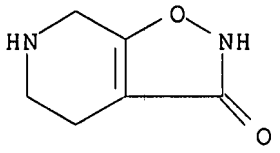
CRN 110-15-6
CMF C4 H6 O4



RN 914291-64-8 CAPLUS
CN Isoxazolo[5,4-c]pyridin-3(2H)-one, 4,5,6,7-tetrahydro-, sulfate (2:1) (9CI) (CA INDEX NAME)

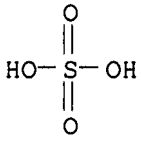
CM 1

CRN 64603-91-4
CMF C6 H8 N2 O2

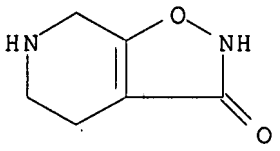


CM 2

CRN 7664-93-9
CMF H2 O4 S

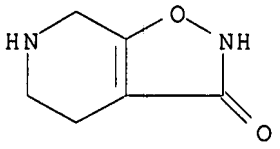


RN 914291-66-0 CAPLUS
CN Isoxazolo[5,4-c]pyridin-3(2H)-one, 4,5,6,7-tetrahydro-, calcium salt (2:1) (9CI) (CA INDEX NAME)



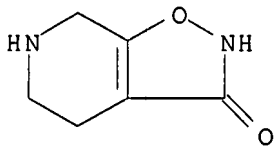
●1/2 Ca

RN 914291-67-1 CAPLUS
CN Isoxazolo[5,4-c]pyridin-3(2H)-one, 4,5,6,7-tetrahydro-, monopotassium salt (9CI) (CA INDEX NAME)



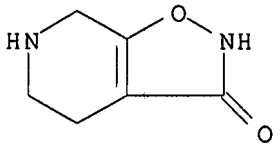
● K

RN 914291-68-2 CAPLUS
CN Isoxazolo[5,4-c]pyridin-3(2H)-one, 4,5,6,7-tetrahydro-, magnesium salt (2:1) (9CI) (CA INDEX NAME)



● 1/2 Mg

RN 914291-69-3 CAPLUS
CN Isoxazolo[5,4-c]pyridin-3(2H)-one, 4,5,6,7-tetrahydro-, monosodium salt (9CI) (CA INDEX NAME)

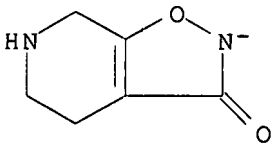


● Na

RN 914291-71-7 CAPLUS
CN Ethanaminium, 2-hydroxy-N,N,N-trimethyl-, salt with 4,5,6,7-tetrahydroisoxazolo[5,4-c]pyridin-3(2H)-one (1:1) (9CI) (CA INDEX NAME)

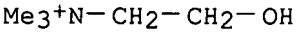
CM 1

CRN 914291-70-6
CMF C6 H7 N2 O2



CM 2

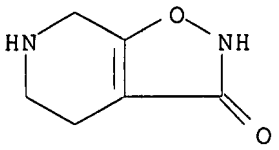
CRN 62-49-7
CMF C5 H14 N O



RN 914291-72-8 CAPLUS
CN L-Lysine, compd. with 4,5,6,7-tetrahydroisoxazolo[5,4-c]pyridin-3(2H)-one (1:1) (9CI) (CA INDEX NAME)

CM 1

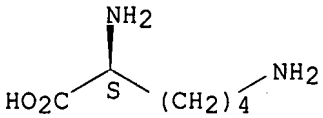
CRN 64603-91-4
CMF C6 H8 N2 O2



CM 2

CRN 56-87-1
CMF C6 H14 N2 O2

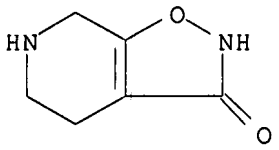
Absolute stereochemistry.



RN 914291-73-9 CAPLUS
CN Isoxazolo[5,4-c]pyridin-3(2H)-one, 4,5,6,7-tetrahydro-, compd. with N,N-bis(phenylmethyl)-1,2-ethanediamine (1:1) (9CI) (CA INDEX NAME)

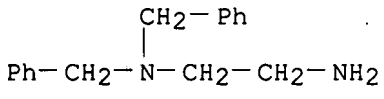
CM 1

CRN 64603-91-4
CMF C6 H8 N2 O2



CM 2

CRN 14165-27-6
CMF C16 H20 N2



REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 2 OF 13 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2006:1009629 CAPLUS
DOCUMENT NUMBER: 145:383399
TITLE: Gaboxadol forms, compositions thereof, methods for preparation and uses for treating sleep disorders
INVENTOR(S): Almarsson, Orn; Hickey, Magali Bourghol; Peterson, Matthew

PATENT ASSIGNEE(S): Transform Pharmaceuticals, Inc., USA
SOURCE: PCT Int. Appl., 56pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2006102093	A1	20060928	WO 2006-US9737	20060317

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW

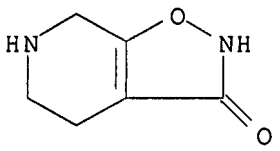
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

PRIORITY APPLN. INFO.: US 2005-663423P P 20050318

AB The invention provides novel gaboxadol forms and methods fo making and using the same. These forms include salts, hydrates, solvates, and polymorphs of gaboxadol with improved aqueous solubility when compared to known gaboxadol forms. The invention also provides novel compns. comprising these novel soluble forms and a suitable carrier. The invention also provides related methods of treatment. Compns. and methods of the invention of the invention have a number of uses, including the treatment or prevention of sleep disorders.

IT 815574-58-4P, Gaboxadol monohydrate 910641-51-9P
RL: PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(gaboxadol forms, compns. thereof, methods for preparation and uses for treating sleep disorders)

RN 815574-58-4 CAPLUS
CN Isoxazolo[5,4-c]pyridin-3(2H)-one, 4,5,6,7-tetrahydro-, monohydrate (9CI) (CA INDEX NAME)

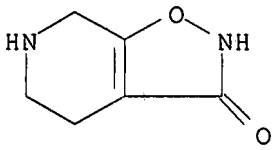


● H_2O

RN 910641-51-9 CAPLUS
CN Isoxazolo[5,4-c]pyridin-3(2H)-one, 4,5,6,7-tetrahydro-, (2Z)-2-butenedioate (9CI) (CA INDEX NAME)

CM 1

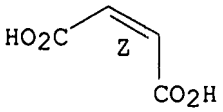
CRN 64603-91-4
CMF C6 H8 N2 O2



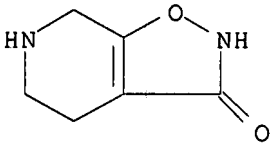
CM 2

CRN 110-16-7
CMF C4 H4 O4

Double bond geometry as shown.



IT 64603-91-4P, Gaboxadol
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(gaboxadol forms, compns. thereof, methods for preparation and uses for treating sleep disorders)
RN 64603-91-4 CAPLUS
CN Isoxazolo[5,4-c]pyridin-3(2H)-one, 4,5,6,7-tetrahydro- (CA INDEX NAME)



REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 3 OF 13 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2006:795633 CAPLUS
DOCUMENT NUMBER: 145:217970
TITLE: Polymorphic forms of a GABA agonist
INVENTOR(S): Kumke, Daniel J.; Murry, Jerry A.; Simmons, Bryon L.; Xu, Feng
PATENT ASSIGNEE(S): Merck & Co., Inc., USA
SOURCE: PCT Int. Appl., 12pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2006083682	A2	20060810	WO 2006-US2809	20060126
WO 2006083682	A3	20070405		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC,

VN, YU, ZA, ZM, ZW
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AP, EA, EP, OA

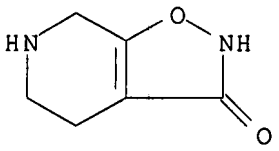
PRIORITY APPLN. INFO.: US 2005-648151P P 20050128

AB The present invention is directed to novel polymorphic forms of 4,5,6,7-tetrahydroisoxazolo[5,4-c]pyridin-3-ol hydrate (gaboxadol monohydrate). The invention is further concerned with pharmaceutical compns. containing the polymorphic forms as an active ingredient, methods for treatment of disorders susceptible to amelioration by GABAA receptor agonism with the polymorphic forms, and processes for the preparation of the polymorphic forms. Gaboxadol-HCl was dissolved in water-isopropanol and was treated with 1 equiv of 5N NaOH. The solution was stirred and the slurry was aged for hours at ambient temperature The resulting white solid was filtered and air dried to give the gaboxadol monohydrate form III.

IT 815574-58-4P, Gaboxadol monohydrate
RL: PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(polymorphic forms of GABA agonist)

RN 815574-58-4 CAPLUS

CN Isoxazolo[5,4-c]pyridin-3(2H)-one, 4,5,6,7-tetrahydro-, monohydrate (9CI) (CA INDEX NAME)



● H_2O

L3 ANSWER 4 OF 13 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2005:686172 CAPLUS
DOCUMENT NUMBER: 143:179592
TITLE: Crystalline forms of a GABAA agonist, gaboxadol for treatment of neurological and psychiatric disorders
INVENTOR(S): Cooper, Vincent Brett
PATENT ASSIGNEE(S): Merck Sharp & Dohme Limited, UK
SOURCE: Brit. UK Pat. Appl., 19 pp.
CODEN: BAXXDU
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
GB 2410434	A	20050803	GB 2005-1847	20050128
US 2005171142	A1	20050804	US 2005-45768	20050128
AU 2005209473	A1	20050811	AU 2005-209473	20050128
CA 2554536	A1	20050811	CA 2005-2554536	20050128
WO 2005073237	A2	20050811	WO 2005-GB288	20050128

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY,

TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

EP 1713813	A2	20061025	EP 2005-702040		20050128
CN 1914212	A	20070214	CN 2005-80003161		20050128
NO 2006003843	A	20060829	NO 2006-3843		20060829
PRIORITY APPLN. INFO.:			GB 2004-2118	A	20040130
			WO 2005-GB288	W	20050128

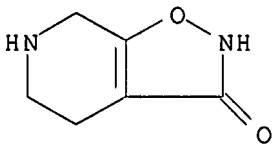
AB Two new crystalline monohydrates and two new crystalline anhydrates of gaboxadol are disclosed together with methods for preparing them. The methods comprise dissolving an acid salt of gaboxadol in water, adjusting the pH to pH 6.5 and either collecting the precipitate immediately or allowing it to age for 12 h.

The crystalline gaboxadol is intended for use in the treatment of neurol. or psychiatric disorders susceptible to amelioration by GABAA receptor agonist. Thus, a solution of gaboxadol hydrochloride was treated with sufficient triethylamine to give a pH of 6.5. The resulting white solid was collected, filtered and air dried giving gaboxadol monohydrate Form I.

IT 815574-58-4P
RL: PNU (Preparation, unclassified); PRP (Properties); RCT (Reactant); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(crystalline forms of gaboxadol for dosage forms for treatment of neurol. or psychiatric disorders susceptible to amelioration by GABAA receptor agonism)

RN 815574-58-4 CAPLUS

CN Isoxazolo[5,4-c]pyridin-3(2H)-one, 4,5,6,7-tetrahydro-, monohydrate (9CI) (CA INDEX NAME)

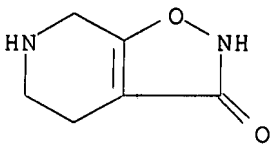


● H_2O

IT 64603-91-4P, Gaboxadol
RL: PNU (Preparation, unclassified); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(crystalline forms of gaboxadol for dosage forms for treatment of neurol. or psychiatric disorders susceptible to amelioration by GABAA receptor agonism)

RN 64603-91-4 CAPLUS

CN Isoxazolo[5,4-c]pyridin-3(2H)-one, 4,5,6,7-tetrahydro- (CA INDEX NAME)



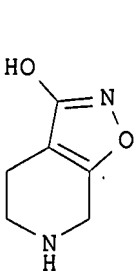
REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 5 OF 13 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2005:238996 CAPLUS
DOCUMENT NUMBER: 142:316828
TITLE: Method for the manufacture of THIP
INVENTOR(S): Petersen, Hans; Bech Sommer, Michael; Dancer, Robert
PATENT ASSIGNEE(S): H. Lundbeck A/S, Den.
SOURCE: PCT Int. Appl., 34 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

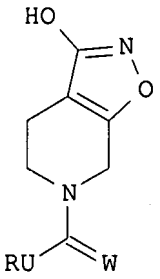
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005023820	A1	20050317	WO 2004-DK579	20040901
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2004270323	A1	20050317	AU 2004-270323	20040901
CA 2537840	A1	20050317	CA 2004-2537840	20040901
EP 1664060	A1	20060607	EP 2004-762799	20040901
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK, HR				
CN 1845928	A	20061011	CN 2004-80025424	20040901
BR 2004013741	A	20061024	BR 2004-13741	20040901
JP 2007504179	T	20070301	JP 2006-525046	20040901
NO 2006001424	A	20060329	NO 2006-1424	20060329

PRIORITY APPLN. INFO.:
DK 2003-1277 A 20030905
US 2003-500422P P 20030905
WO 2004-DK579 W 20040901

OTHER SOURCE(S): CASREACT 142:316828; MARPAT 142:316828
GI



I



II

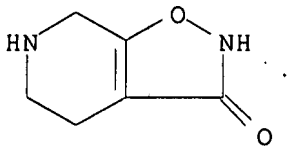
AB The present invention relates to a new method of preparing gaboxadol (THIP; I), which is useful for treating sleep disorders (no data). In particular a method of preparing THIP comprising reacting a compound II [R = alkyl, cycloalkyl, aryl, etc.; U = N, CR1 (R1 = H, R); W = O, S, NR4 (R4 = H, R)]

or a salt thereof with an acid, typically a mineral acid, to obtain THIP as an acid addition salt. The present invention also relates to several intermediates. E.g., a multi-step synthesis of I.HBr, starting from Me 3-hydroxyisonicotinate, was given.

IT 65202-63-3P
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
(method for the manufacture of THIP)

RN 65202-63-3 CAPLUS

CN Isoxazolo[5,4-c]pyridin-3(2H)-one, 4,5,6,7-tetrahydro-, monohydrobromide (9CI) (CA INDEX NAME)



● HBr

REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 6 OF 13 CAPLUS COPYRIGHT 2007 ACS on STN

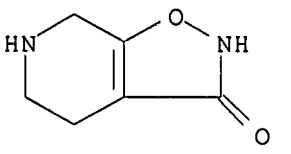
ACCESSION NUMBER: 2004:720824 CAPLUS
DOCUMENT NUMBER: 141:306879
TITLE: Gaboxadol (Lundbeck/Merck)
AUTHOR(S): Huckle, Richard
CORPORATE SOURCE: Innovation Center, Actelion Ltd, Allschwil, CH-4123, Switz.
SOURCE: Current Opinion in Investigational Drugs (Thomson Scientific) (2004), 5(7), 766-773
CODEN: COIDAZ; ISSN: 1472-4472
PUBLISHER: Thomson Scientific
DOCUMENT TYPE: Journal; General Review
LANGUAGE: English

AB A review. H Lundbeck A/S, in collaboration with Merck & Co Inc, is developing gaboxadol, a GABAA agonist, for the potential treatment of sleep disorders. The compound is currently undergoing phase III clin. trials.

IT 64603-91-4P, Gaboxadol
RL: ADV (Adverse effect, including toxicity); DMA (Drug mechanism of action); PAC (Pharmacological activity); PKT (Pharmacokinetics); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(GABAA agonist gaboxadol for potential treatment of sleep disorders)

RN 64603-91-4 CAPLUS

CN Isoxazolo[5,4-c]pyridin-3(2H)-one, 4,5,6,7-tetrahydro- (CA INDEX NAME)



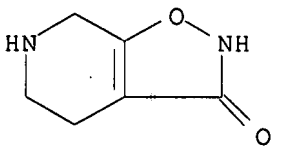
REFERENCE COUNT: 64 THERE ARE 64 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 7 OF 13 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1995:726673 CAPLUS
DOCUMENT NUMBER: 123:169581
TITLE: Partial GABAA Receptor Agonists. Synthesis and in Vitro Pharmacology of a Series of Nonannulated Analogs of 4,5,6,7-Tetrahydroisoxazolo[4,5-c]pyridin-3-ol
AUTHOR(S): Frolund, Bente; Kristiansen, Uffe; Brehm, Lotte; Hansen, Annette B.; Krogsgaard-Larsen, Povl; Falch, Erik
CORPORATE SOURCE: PharmaBiotec Research Center, Royal Danish School of Pharmacy, Copenhagen, DK-2100, Den.
SOURCE: Journal of Medicinal Chemistry (1995), 38(17), 3287-96
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 123:169581

AB 5-(4-Piperidinyl)3-isoxazolol (4-PIOL), a structural analog of 4-aminobutanoic acid (GABA) and the GABAA agonist 4,5,6,7-tetrahydroisoxazolo[5,4-c]pyridin-3-ol (THIP), is a low-efficacy partial GABAA agonist. A number of compds. bioisosterically derived from 4-PIOL, including 5-(4-piperidinyl)-3-isothiazolol, 3-(4-piperidinyl)-5-isoxazolol 5-(1,2,3,6-tetrahydropyrid-4-yl)-3-isoxazolol, and 5-(1,2,3,6-tetrahydropyrid-4-yl)isothiazol-3-ol, were synthesized and tested as GABAA receptor ligands. Whereas none of these compds. significantly affected GABAB receptor binding or GABA uptake, they showed affinities for GABAA receptor sites in the low-micromolar range. Using cultured cerebral cortical neurons and whole-cell patch-clamp techniques, the efficacies of these compds. relative to that of the full GABAA agonist, isoguvacine (20 μM), were determined The relative efficacy of 5-(4-piperidinyl)-3-isothiazolol , which has a higher receptor affinity (IC50 = 1.3 μM) than 4-PIOL (IC50 = 9.3 μM), was comparable with that of 4-PIOL (30-35%). The tetrahydropyridine analog of 4-PIOL, compound 5-(1,2,3,6-tetrahydropyrid-4-yl)-3-isoxazolol, showed a markedly lower receptor affinity (IC50 = 32 μM) and apparently a lower relative efficacy than 4-PIOL. The corresponding unsatd. analog of 5-(4-piperidinyl)-3-isothiazolol , compound 14, showed a slightly weaker receptor affinity (IC50 = 4.0 μM) but a significantly higher relative efficacy (50-55%) than 5-(4-piperidinyl)-3-isothiazolol . The 5-isoxazolol isomer of 4-PIOL, compound 3-(4-piperidinyl)-5-isoxazolol , showed a reduced receptor affinity (IC50 = 26 μM) and a very low relative efficacy. Substitution of propanoic or propenoic acid moieties for the acidic heterocyclic units of these compds. gave the monocyclic amino acid derivs., which have very little or no affinity for GABAA receptor sites.

IT 64603-91-4DP, Isoxazolo[5,4-c]pyridin-3(2H)-one, 4,5,6,7-tetrahydro, analogs
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(THIP; preparation of isoxazolo[5,4-c]pyridinone analogs as GABAa agonists)
RN 64603-91-4 CAPLUS
CN Isoxazolo[5,4-c]pyridin-3(2H)-one, 4,5,6,7-tetrahydro- (CA INDEX NAME)



L3 ANSWER 8 OF 13 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1992:591577 CAPLUS
DOCUMENT NUMBER: 117:191577

TITLE: 3-Hydroxyisoxazole bioisosteres of GABA. Synthesis of a series of 4-substituted muscimol analogs and identification of a bicyclic 2-isoxazoline rearrangement product

AUTHOR(S): Hjeds, Hans; Christensen, Inge T.; Cornett, Claus; Froelund, Bente; Falch, Erik; Pedersen, Joergen B.; Krogsgaard-Larsen, Povl

CORPORATE SOURCE: PharmaBiotec Res. Cent., R. Dan. Sch. Pharm., Copenhagen, DK-2100, Den.

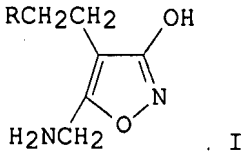
SOURCE: Acta Chemica Scandinavica (1992), 46(8), 772-7
CODEN: ACHSE7; ISSN: 0904-213X

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 117:191577

GI



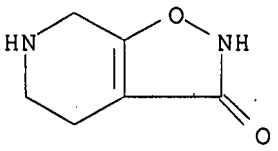
I

AB 3-Hydroxy-4-(2-hydroxyethyl)-5-methylisoxazole was used as the starting material for the syntheses of the muscimol analogs I (R = OH, Cl, OAc). Whilst muscimol is a very potent agonist at GABAA receptors, I did not show significant affinity for GABAA receptor sites in vitro.

IT 65202-63-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 65202-63-3 CAPLUS

CN Isoxazolo[5,4-c]pyridin-3(2H)-one, 4,5,6,7-tetrahydro-, monohydrobromide (9CI) (CA INDEX NAME)



● HBr

L3 ANSWER 9 OF 13 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1984:465548 CAPLUS

DOCUMENT NUMBER: 101:65548

TITLE: Analgesic GABA agonists. Synthesis and structure-activity studies on analogs and derivatives of muscimol and THIP

AUTHOR(S): Haefliger, Walter; Revesz, Laszlo; Maurer, Richard; Roemer, Dietmar; Buescher, Heinz Hermann

CORPORATE SOURCE: Sandoz Ltd., Basel, CH-4002, Switz.

SOURCE: European Journal of Medicinal Chemistry (1984), 19(2), 149-56
CODEN: EJMCA5; ISSN: 0009-4374

DOCUMENT TYPE: Journal

LANGUAGE: English

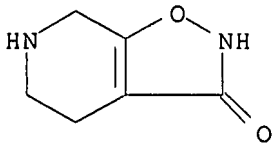
OTHER SOURCE(S): CASREACT 101:65548

AB A series of analogs. and derivs. (prodrugs) of muscimol and THIP were prepared and their GABA receptor affinity, analgesic, and GABAergic properties examined Some compds. designed as prodrugs exhibited high GABA receptor affinity indicating that nonzwitterionic mols. interact with GABA receptors. Analgesic and GABAergic activities of muscimol prodrugs were pronounced but weaker than muscimol itself. A ring opened THIP derivative was inactive whereas its carbamate derivative showed analgesic and GABAergic activity. A benzophenone-imine derivative showed strong GABA binding but no analgesic activity. Carbamate type THIP prodrugs were also active in analgesic and anticonvulsive tests but weaker than THIP itself. Ester- and alkanoyloxymethyl prodrugs were only active in the hot plate test. When the inactive 7-methyl-THIP was converted to a potential prodrug it produced high GABA-mimetic activity in both anticonvulsant and analgesic tests. In all cases, sedation was inseperable from analgesia.

IT 64603-91-4DP, derivs.
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and GABA agonist activity of, mol. structure in relation to)

RN 64603-91-4 CAPLUS

CN Isoxazolo[5,4-c]pyridin-3(2H)-one, 4,5,6,7-tetrahydro- (CA INDEX NAME)



L3 ANSWER 10 OF 13 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1982:562964 CAPLUS

DOCUMENT NUMBER: 97:162964

TITLE: Isoxazolo[5,4-c]pyridines which are GABA-agonists

INVENTOR(S): Krogsgaard-Larsen, Povl

PATENT ASSIGNEE(S): Lundbeck, H., og Co. A/S, Den.

SOURCE: Can., 29 pp. Division of Can. Appl. No. 305,798.
CODEN: CAXXA4

DOCUMENT TYPE: Patent

LANGUAGE: English

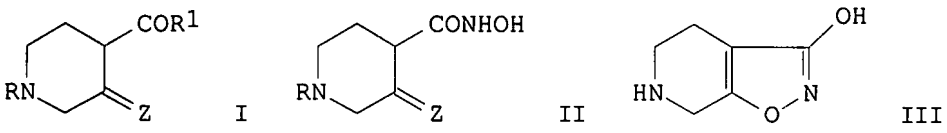
FAMILY ACC. NUM. COUNT: 3

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
CA 1125288	A2	19820608	CA 1981-377128		19810507
CA 1107736	A1	19810825	CA 1978-305798		19780620
US 4301287	A	19811117	US 1979-104080		19791217
PRIORITY APPLN. INFO.:			GB 1977-25740	A	19770620
			CA 1978-305798	A3	19780620
			US 1978-917118	A3	19780619

OTHER SOURCE(S): MARPAT 97:162964

GI

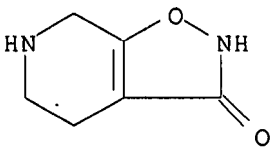


AB Piperidinecarboxylic acid compds. I (R = Ac, carbalkoxy, carbophenoxy, CPh3, CHO; Z = ketalized O; R1 = halo, OH, alkoxy) reacted with HONH2 to

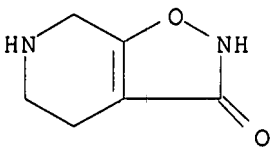
yield hydroxamic acids II. Isoxazolo[5,4-c]pyridine derivative III, which is an agonist of H2N(CH2)3CO2H, was prepared from II. I (R = CO2Me, R1 = OEt, Z = OCH2CH2O) reacted with HONH2 to give II (R = CO2Me, Z = OCH2CH2O), and the latter was treated with HCl and then with HBr-HOAc to give III.HBr.

IT 64603-91-4P 65202-63-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and use of, as gamma-aminobutyric acid agonist)

RN 64603-91-4 CAPLUS
CN Isoxazolo[5,4-c]pyridin-3(2H)-one, 4,5,6,7-tetrahydro- (CA INDEX NAME)



RN 65202-63-3 CAPLUS
CN Isoxazolo[5,4-c]pyridin-3(2H)-one, 4,5,6,7-tetrahydro-, monohydrobromide (9CI) (CA INDEX NAME)

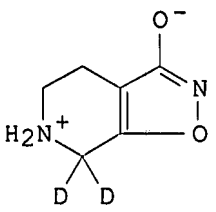


● HBr

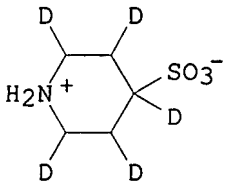
L3 ANSWER 11 OF 13 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER:	1982:527546 CAPLUS
DOCUMENT NUMBER:	97:127546
TITLE:	Deuterium labeling of the GABA agonists THIP, piperidine-4-sulfonic acid, and the GABA uptake inhibitor THPO
AUTHOR(S):	Krogsgaard-Larsen, Povl; Johansen, Joergen Stage; Falch, Erik
CORPORATE SOURCE:	Dep. Chem. BC, R. Dan. Sch. Pharm., Copenhagen, DK-2100, Den.
SOURCE:	Journal of Labelled Compounds and Radiopharmaceuticals (1982), 19(5), 689-702 CODEN: JLCRD4; ISSN: 0362-4803
DOCUMENT TYPE:	Journal
LANGUAGE:	English

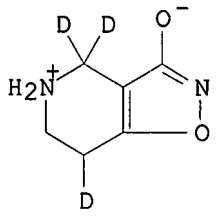
GI



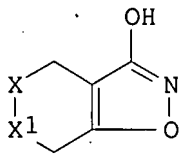
I



II



III



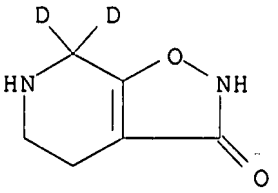
IV

AB The D-labeled title compds. (I, II , and III, resp.) were prepared I and III were prepared from IV (X = CH2, X1 = NCO2Me; X = NCO2Me, X1 = CH2), resp., by sequential methylation, N-decarboxylation, nitrosation, H-D exchange reaction with D2O (acid- and base-catalyzed, resp.), denitrosation, and demethylation. Pt-catalyzed deuteration of pyridine-4-sulfonic acid in D2O gave II.

IT 82988-63-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 82988-63-4 CAPLUS

CN Isoxazolo[5,4-c]pyridin-3(2H)-one-7-d, 4,5,6,7-tetrahydro-7-d- (9CI) (CA INDEX NAME)



L3 ANSWER 12 OF 13 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1979:439458 CAPLUS

DOCUMENT NUMBER: 91:39458

TITLE: Methyl tetrahydrohydroxy isoxazolopyridine carboxylate

INVENTOR(S): Krogsgaard-Larsen, Povl

PATENT ASSIGNEE(S): Den.

SOURCE: Jpn. Kokai Tokkyo Koho, 13 pp.
CODEN: JKXXAF

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 3

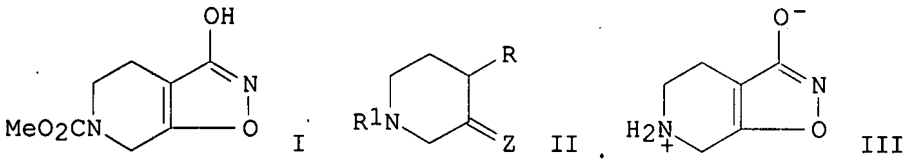
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 54036290	A	19790316	JP 1978-74800	19780620
DK 7802702	A	19781221	DK 1978-2702	19780615
DK 7802703	A	19781221	DK 1978-2703	19780615
FI 7801954	A	19781221	FI 1978-1954	19780619
FI 64376	B	19830729		
FI 64376	C	19831110		
FI 7801955	A	19781221	FI 1978-1955	19780619
NO 7802127	A	19781221	NO 1978-2127	19780619

NO 152049	B	19850415			
NO 152449	C	19850724			
NO 7802128	A	19781221	NO 1978-2128		19780619
EP 167	A1	19790110	EP 1978-100190		19780619
R: BE, CH, DE, FR, GB, LU, NL, SE					
EP 338	A2	19790124	EP 1978-100191		19780619
EP 338	A3	19790627			
EP 338	B1	19811125			
R: BE, CH, DE, FR, GB, LU, NL, SE					
ES 470912	A1	19790201	ES 1978-470912		19780619
ES 470913	A1	19790201	ES 1978-470913		19780619
ZA 7803492	A	19790627	ZA 1978-3492		19780619
ZA 7803493	A	19790627	ZA 1978-3493		19780619
AU 7837244	A	19800103	AU 1978-37244		19780619
US 4278676	A	19810714	US 1978-917118		19780619
AU 7837298	A	19800103	AU 1978-37298		19780620
AU 521040	B2	19820311			
AT 7804486	A	19820215	AT 1978-4486		19780620
AT 368505	B	19821025			
NO 7902839	A	19781221	NO 1979-2839		19790903
US 4301287	A	19811117	US 1979-104080		19791217
EP 27279	A1	19810422	EP 1980-106497		19801023
R: BE, CH, DE, FR, GB, LU, NL, SE					
EP 28017	A1	19810506	EP 1980-106498		19801023
R: BE, CH, DE, FR, GB, LU, NL, SE					
PRIORITY APPLN. INFO.:			GB 1977-25740	A	19770620
			US 1978-917118	A3	19780619

OTHER SOURCE(S): MARPAT 91:39458

GI

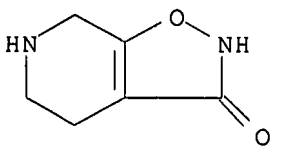


AB The title compound (I) was prepared Thus, (methoxycarbonyl)piperidinone II (R = CO2Et, R1 = CO2Me, Z = O) [obtained by hydrogenating II (R = CO2Et, R1 = CH2Ph, Z = O) over Pd-C, and reacting the product with ClCO2Me] was ketalized with HOCH2CH2OH to give the ethylene acetal II (R = CO2Et, R1 = CO2Me, Z = OCH2CH2O), which was treated with H2NOH.HCl to give II (R = CONHOH, R1 = CO2Me, Z = OCH2CH2O), whose cyclization in H2SO4 gave the hydroxyisoxazolopiperidinecarboxylate. Decarboxylation of I followed by treatment with HBr and then H2O-Et3N-EtOH gave zwitterion III. III was a mild tranquilizer in mice.

IT 64603-91-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and tranquilizing activity of)

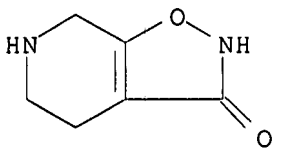
RN 64603-91-4 CAPLUS

CN Isoxazolo[5,4-c]pyridin-3(2H)-one, 4,5,6,7-tetrahydro- (CA INDEX NAME)



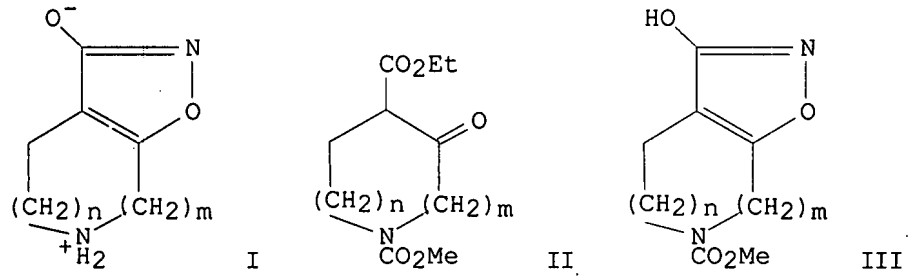
IT 65202-63-3P
RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of)
RN 65202-63-3 CAPLUS
CN Isoxazolo[5,4-c]pyridin-3(2H)-one, 4,5,6,7-tetrahydro-, monohydrobromide (9CI) (CA INDEX NAME)



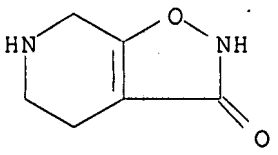
● HBr

L3 ANSWER 13 OF 13 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1978:37672 CAPLUS
DOCUMENT NUMBER: 88:37672
TITLE: Muscimol analogs. II. Synthesis of some bicyclic 3-isoxazolol zwitterions
AUTHOR(S): Krogsgaard-Larsen, Povl
CORPORATE SOURCE: Dep. Chem. BC, R. Dan. Sch. Pharm., Copenhagen, Den.
SOURCE: Acta Chemica Scandinavica, Series B: Organic Chemistry and Biochemistry (1977), B31(7), 584-8
CODEN: ACBOCV; ISSN: 0302-4369
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 88:37672
GI



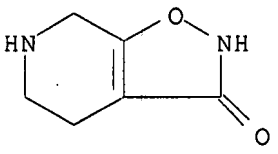
I II III

AB The 3-isoxazolol zwitterions 4,5,6,7-tetrahydroisoxazolo[5,4-c]pyridin-3-ol, (I, n = 1, m = 1), 5,6,7,8-tetrahydro-4H-isoxazolo[5,4-c]azepin-3-ol (I, n = 2, m = 1), and 5,6,7,8-tetrahydro-4H-isoxazolo[4,5-c]azepin-3-ol (I, n = o, m = 3) were prepared The starting materials were the cyclic β-oxoesters II. The ethylene acetals of II were treated with HONH2 followed by deacetalization and cyclization of the intermediate β-oxohydroxamic acid ethylene acetals to give the resp. 3-isoxazolol derivs. III, which were transformed into the zwitterions I. The pKA values of I were determined
IT 65202-63-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction with triethylamine, zwitterions from)
RN 65202-63-3 CAPLUS
CN Isoxazolo[5,4-c]pyridin-3(2H)-one, 4,5,6,7-tetrahydro-, monohydrobromide (9CI) (CA INDEX NAME)



● HBr

IT 64603-91-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 64603-91-4 CAPLUS
CN Isoxazolo[5,4-c]pyridin-3(2H)-one, 4,5,6,7-tetrahydro- (CA INDEX NAME)



=> FIL STNGUIDE

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	74.41	249.18
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-10.14	-10.14

FILE 'STNGUIDE' ENTERED AT 12:44:01 ON 09 MAY 2007

FILE CONTAINS CURRENT INFORMATION.
LAST RELOADED: May 4, 2007 (20070504/UP).

=> s l3 and leav?
COMBINATION OF STRUCTURE AND TEXT TERMS NOT VALID
The query entered contains both search terms created by structure-building or screen commands and text search terms. L#s created via the STRUCTURE or SCREEN commands must be searched in the structures files separately from text terms or profiles. The L# answer sets from structure searches can be used in crossover searches and can be combined with text terms.

=> s l3 and leav?
COMBINATION OF STRUCTURE AND TEXT TERMS NOT VALID
The query entered contains both search terms created by structure-building or screen commands and text search terms. L#s created via the STRUCTURE or SCREEN commands must be searched in the structures files separately from text terms or profiles. The L# answer sets from structure searches can be used in crossover searches and can be combined with text terms.

=> file caplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION

FULL ESTIMATED COST 0.48 249.66

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE ENTRY TOTAL SESSION
CA SUBSCRIBER PRICE 0.00 -10.14

FILE 'CAPLUS' ENTERED AT 12:48:41 ON 09 MAY 2007
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

FILE COVERS 1907 - 9 May 2007 VOL 146 ISS 20
FILE LAST UPDATED: 8 May 2007 (20070508/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply. They are available for your review at:

http://www.cas.org/infopolicy.html

```
=> s l3 and leav?
        277799 LEAV?
L5           0 L3 AND LEAV?

=> s l3
           481 L2
       4400083 PREP/RL
L6          13 L2/PREP
                 (L2 (L) PREP/RL)

=> s l6 and leav?
        277799 LEAV?
L7           0 L6 AND LEAV?

=> s l6 and react?
       4932193 REACT?
L8           8 L6 AND REACT?

=> d ibib abs hitstr tot

L8   ANSWER 1 OF 8  CAPLUS  COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER:        2006:1009629  CAPLUS
DOCUMENT NUMBER:         145:383399
TITLE:                   Gaboxadol forms, compositions thereof, methods for
                         preparation and uses for treating sleep disorders
INVENTOR(S):             Almarsson, Orn; Hickey, Magali Bourghol; Peterson,
                         Matthew
PATENT ASSIGNEE(S):      Transform Pharmaceuticals, Inc., USA
SOURCE:                  PCT Int. Appl., 56pp.
                         CODEN: PIXXD2
DOCUMENT TYPE:           Patent
LANGUAGE:                English
FAMILY ACC. NUM. COUNT:  1
PATENT INFORMATION:
```

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2006102093	A1	20060928	WO 2006-US9737	20060317

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW

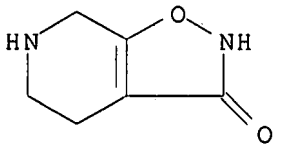
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

PRIORITY APPLN. INFO.: US 2005-663423P P 20050318

AB The invention provides novel gaboxadol forms and methods fo making and using the same. These forms include salts, hydrates, solvates, and polymorphs of gaboxadol with improved aqueous solubility when compared to known gaboxadol forms. The invention also provides novel compns. comprising these novel soluble forms and a suitable carrier. The invention also provides related methods of treatment. Compns. and methods of the invention of the invention have a number of uses, including the treatment or prevention of sleep disorders.

IT 815574-58-4P, Gaboxadol monohydrate 910641-51-9P
RL: PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(gaboxadol forms, compns. thereof, methods for preparation and uses for treating sleep disorders)

RN 815574-58-4 CAPLUS
CN Isoxazolo[5,4-c]pyridin-3(2H)-one, 4,5,6,7-tetrahydro-, monohydrate (9CI) (CA INDEX NAME)

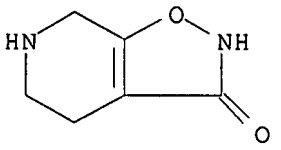


● H_2O

RN 910641-51-9 CAPLUS
CN Isoxazolo[5,4-c]pyridin-3(2H)-one, 4,5,6,7-tetrahydro-, (2Z)-2-butenedioate (9CI) (CA INDEX NAME)

CM 1

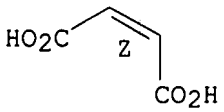
CRN 64603-91-4
CMF C6 H8 N2 O2



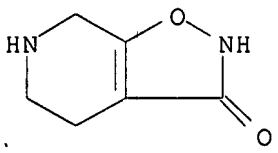
CM 2

CRN 110-16-7
CMF C4 H4 O4

Double bond geometry as shown.



IT 64603-91-4P, Gaboxadol
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(gaboxadol forms, compns. thereof, methods for preparation and uses for treating sleep disorders)
RN 64603-91-4 CAPLUS
CN Isoxazolo[5,4-c]pyridin-3(2H)-one, 4,5,6,7-tetrahydro- (CA INDEX NAME)



REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 2 OF 8 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2006:795633 CAPLUS
DOCUMENT NUMBER: 145:217970
TITLE: Polymorphic forms of a GABA agonist
INVENTOR(S): Kumke, Daniel J.; Murry, Jerry A.; Simmons, Bryon L.; Xu, Feng
PATENT ASSIGNEE(S): Merck & Co., Inc., USA
SOURCE: PCT Int. Appl., 12pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2006083682	A2	20060810	WO 2006-US2809	20060126
WO 2006083682	A3	20070405		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AP, EA, EP, OA

PRIORITY APPLN. INFO.: US 2005-648151P P 20050128

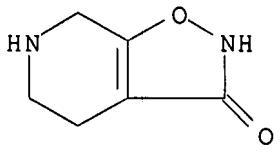
AB The present invention is directed to novel polymorphic forms of 4,5,6,7-tetrahydroisoxazolo[5,4-c]pyridin-3-ol hydrate (gaboxadol monohydrate). The invention is further concerned with pharmaceutical

compns. containing the polymorphic forms as an active ingredient, methods for treatment of disorders susceptible to amelioration by GABAA receptor agonism with the polymorphic forms, and processes for the preparation of the polymorphic forms. Gaboxadol-HCl was dissolved in water-isopropanol and was treated with 1 equiv of 5N NaOH. The solution was stirred and the slurry was aged for hours at ambient temperature The resulting white solid was filtered and air dried to give the gaboxadol monohydrate form III.

IT 815574-58-4P, Gaboxadol monohydrate
RL: PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(polymorphic forms of GABA agonist)

RN 815574-58-4 CAPLUS

CN Isoxazolo[5,4-c]pyridin-3(2H)-one, 4,5,6,7-tetrahydro-, monohydrate (9CI) (CA INDEX NAME)



● H_2O

L8 ANSWER 3 OF 8 CAPLUS COPYRIGHT 2007 ACS on STN

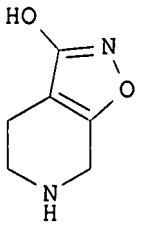
ACCESSION NUMBER: 2005:238996 CAPLUS
DOCUMENT NUMBER: 142:316828
TITLE: Method for the manufacture of THIP
INVENTOR(S): Petersen, Hans; Bech Sommer, Michael; Dancer, Robert
PATENT ASSIGNEE(S): H. Lundbeck A/S, Den.
SOURCE: PCT Int. Appl., 34 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005023820	A1	20050317	WO 2004-DK579	20040901
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2004270323	A1	20050317	AU 2004-270323	20040901
CA 2537840	A1	20050317	CA 2004-2537840	20040901
EP 1664060	A1	20060607	EP 2004-762799	20040901
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK, HR				
CN 1845928	A	20061011	CN 2004-80025424	20040901
BR 2004013741	A	20061024	BR 2004-13741	20040901
JP 2007504179	T	20070301	JP 2006-525046	20040901
NO 2006001424	A	20060329	NO 2006-1424	20060329

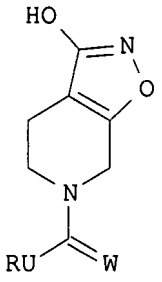
PRIORITY APPLN. INFO.: DK 2003-1277 A 20030905
US 2003-500422P P 20030905
WO 2004-DK579 W 20040901

OTHER SOURCE(S): CASREACT 142:316828; MARPAT 142:316828

GI



I



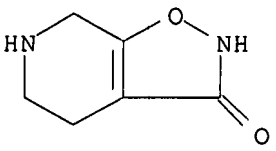
II

AB The present invention relates to a new method of preparing gaboxadol (THIP; I), which is useful for treating sleep disorders (no data). In particular a method of preparing THIP comprising reacting a compound II [R = alkyl, cycloalkyl, aryl, etc.; U = N, CR1 (R1 = H, R); W = O, S, NR4 (R4 = H, R)] or a salt thereof with an acid, typically a mineral acid, to obtain THIP as an acid addition salt. The present invention also relates to several intermediates. E.g., a multi-step synthesis of I.HBr, starting from Me 3-hydroxyisonicotinate, was given.

IT 65202-63-3P
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
(method for the manufacture of THIP)

RN 65202-63-3 CAPLUS

CN Isoxazolo[5,4-c]pyridin-3(2H)-one, 4,5,6,7-tetrahydro-, monohydrobromide (9CI) (CA INDEX NAME)



● HBr

REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

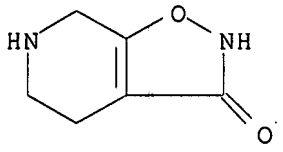
L8 ANSWER 4 OF 8 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1984:465548 CAPLUS
DOCUMENT NUMBER: 101:65548
TITLE: Analgesic GABA agonists. Synthesis and structure-activity studies on analogs and derivatives of muscimol and THIP
AUTHOR(S): Haefliger, Walter; Revesz, Laszlo; Maurer, Richard; Roemer, Dietmar; Buescher, Heinz Hermann
CORPORATE SOURCE: Sandoz Ltd., Basel, CH-4002, Switz.
SOURCE: European Journal of Medicinal Chemistry (1984), 19(2), 149-56
CODEN: EJMCA5; ISSN: 0009-4374

DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 101:65548

AB A series of analogs. and derivs. (prodrugs) of muscimol and THIP were prepared and their GABA receptor affinity, analgesic, and GABAergic properties examined Some compds. designed as prodrugs exhibited high GABA receptor affinity indicating that nonzwitterionic mols. interact with GABA receptors. Analgesic and GABAergic activities of muscimol prodrugs were pronounced but weaker than muscimol itself. A ring opened THIP derivative was inactive whereas its carbamate derivative showed analgesic and GABAergic activity. A benzophenone-imine derivative showed strong GABA binding but no analgesic activity. Carbamate type THIP prodrugs were also active in analgesic and anticonvulsive tests but weaker than THIP itself. Ester- and alkanoyloxymethyl prodrugs were only active in the hot plate test. When the inactive 7-methyl-THIP was converted to a potential prodrug it produced high GABA-mimetic activity in both anticonvulsant and analgesic tests. In all cases, sedation was inseperable from analgesia.

IT 64603-91-4DP, derivs.
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and GABA agonist activity of, mol. structure in relation to)

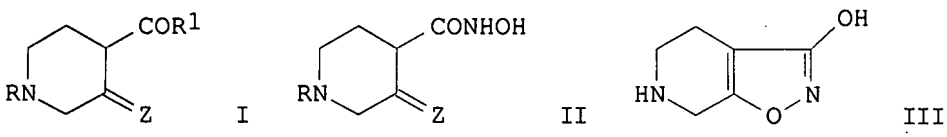
RN 64603-91-4 CAPLUS
CN Isoxazolo[5,4-c]pyridin-3(2H)-one, 4,5,6,7-tetrahydro- (CA INDEX NAME)



L8 ANSWER 5 OF 8 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1982:562964 CAPLUS
DOCUMENT NUMBER: 97:162964
TITLE: Isoxazolo[5,4-c]pyridines which are GABA-agonists
INVENTOR(S): Krogsgaard-Larsen, Povl
PATENT ASSIGNEE(S): Lundbeck, H., og Co. A/S, Den.
SOURCE: Can., 29 pp. Division of Can. Appl. No. 305,798.
CODEN: CAXXA4
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
CA 1125288	A2	19820608	CA 1981-377128		19810507
CA 1107736	A1	19810825	CA 1978-305798		19780620
US 4301287	A	19811117	US 1979-104080		19791217
PRIORITY APPLN. INFO.:			GB 1977-25740	A	19770620
			CA 1978-305798	A3	19780620
			US 1978-917118	A3	19780619

OTHER SOURCE(S): MARPAT 97:162964
GI

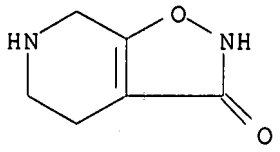


AB Piperidinecarboxylic acid compds. I (R = Ac, carbalkoxy, carbophenoxy, CPh3, CHO; Z = ketalized O; R1 = halo, OH, alkoxy) reacted with HONH2 to yield hydroxamic acids II. Isoxazolo[5,4-c]pyridine derivative III, which is an agonist of H2N(CH2)3CO2H, was prepared from II. I (R = CO2Me, R1 = OEt, Z = OCH2CH2O) reacted with HONH2 to give II (R = CO2Me, Z = OCH2CH2O), and the latter was treated with HCl and then with HBr-HOAc to give III.HBr.

IT 64603-91-4P 65202-63-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and use of, as gamma-aminobutyric acid agonist)

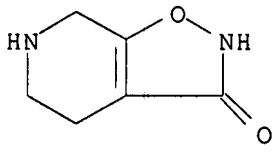
RN 64603-91-4 CAPLUS

CN Isoxazolo[5,4-c]pyridin-3(2H)-one, 4,5,6,7-tetrahydro- (CA INDEX NAME)



RN 65202-63-3 CAPLUS

CN Isoxazolo[5,4-c]pyridin-3(2H)-one, 4,5,6,7-tetrahydro-, monohydrobromide (9CI) (CA INDEX NAME)



● HBr

L8 ANSWER 6 OF 8 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1982:527546 CAPLUS

DOCUMENT NUMBER: 97:127546

TITLE: Deuterium labeling of the GABA agonists THIP, piperidine-4-sulfonic acid, and the GABA uptake inhibitor THPO

AUTHOR(S): Krogsgaard-Larsen, Povl; Johansen, Joergen Stage; Falch, Erik

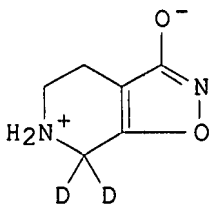
CORPORATE SOURCE: Dep. Chem. BC, R. Dan. Sch. Pharm., Copenhagen, DK-2100, Den.

SOURCE: Journal of Labelled Compounds and Radiopharmaceuticals (1982), 19(5), 689-702
CODEN: JLCRD4; ISSN: 0362-4803

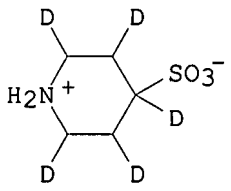
DOCUMENT TYPE: Journal

LANGUAGE: English

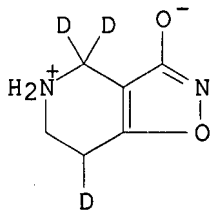
GI



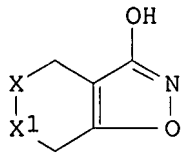
I



II



III



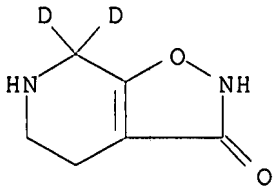
IV

AB The D-labeled title compds. (I, II , and III, resp.) were prepared I and III were prepared from IV (X = CH2, X1 = NCO2Me; X = NCO2Me, X1 = CH2), resp., by sequential methylation, N-decarboxylation, nitrosation, H-D exchange reaction with D2O (acid- and base-catalyzed, resp.), denitrosation, and demethylation. Pt-catalyzed deuteration of pyridine-4-sulfonic acid in D2O gave II.

IT 82988-63-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 82988-63-4 CAPLUS

CN Isoxazolo[5,4-c]pyridin-3(2H)-one-7-d, 4,5,6,7-tetrahydro-7-d- (9CI) (CA INDEX NAME)



L8 ANSWER 7 OF 8 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1979:439458 CAPLUS

DOCUMENT NUMBER: 91:39458

TITLE: Methyl tetrahydrohydroxy isoxazolopyridine carboxylate

INVENTOR(S): Krogsgaard-Larsen, Povl

PATENT ASSIGNEE(S): Den.

SOURCE: Jpn. Kokai Tokkyo Koho, 13 pp.
CODEN: JKXXAF

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 3

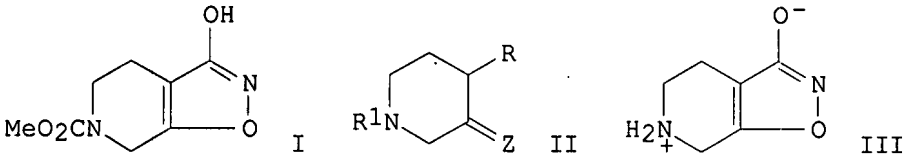
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 54036290	A	19790316	JP 1978-74800	19780620
DK 7802702	A	19781221	DK 1978-2702	19780615
DK 7802703	A	19781221	DK 1978-2703	19780615
FI 7801954	A	19781221	FI 1978-1954	19780619
FI 64376	B	19830729		
FI 64376	C	19831110		
FI 7801955	A	19781221	FI 1978-1955	19780619
NO 7802127	A	19781221	NO 1978-2127	19780619

NO 152049	B	19850415			
NO 152449	C	19850724			
NO 7802128	A	19781221	NO 1978-2128		19780619
EP 167	A1	19790110	EP 1978-100190		19780619
R: BE, CH, DE, FR, GB, LU, NL, SE					
EP 338	A2	19790124	EP 1978-100191		19780619
EP 338	A3	19790627			
EP 338	B1	19811125			
R: BE, CH, DE, FR, GB, LU, NL, SE					
ES 470912	A1	19790201	ES 1978-470912		19780619
ES 470913	A1	19790201	ES 1978-470913		19780619
ZA 7803492	A	19790627	ZA 1978-3492		19780619
ZA 7803493	A	19790627	ZA 1978-3493		19780619
AU 7837244	A	19800103	AU 1978-37244		19780619
US 4278676	A	19810714	US 1978-917118		19780619
AU 7837298	A	19800103	AU 1978-37298		19780620
AU 521040	B2	19820311			
AT 7804486	A	19820215	AT 1978-4486		19780620
AT 368505	B	19821025			
NO 7902839	A	19781221	NO 1979-2839		19790903
US 4301287	A	19811117	US 1979-104080		19791217
EP 27279	A1	19810422	EP 1980-106497		19801023
R: BE, CH, DE, FR, GB, LU, NL, SE					
EP 28017	A1	19810506	EP 1980-106498		19801023
R: BE, CH, DE, FR, GB, LU, NL, SE					
PRIORITY APPLN. INFO.:			GB 1977-25740	A	19770620
			US 1978-917118	A3	19780619

OTHER SOURCE(S): MARPAT 91:39458

GI



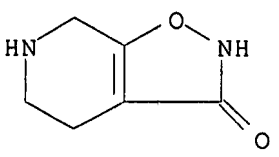
I II III

AB The title compound (I) was prepared Thus, (methoxycarbonyl)piperidinone II (R = CO2Et, R1 = CO2Me, Z = O) [obtained by hydrogenating II (R = CO2Et, R1 = CH2Ph, Z = O) over Pd-C, and reacting the product with ClCO2Me] was ketalized with HOCH2CH2OH to give the ethylene acetal II (R = CO2Et, R1 = CO2Me, Z = OCH2CH2O), which was treated with H2NOH.HCl to give II (R = CONHOH, R1 = CO2Me, Z = OCH2CH2O), whose cyclization in H2SO4 gave the hydroxyisoxazolopiperidinecarboxylate. Decarboxylation of I followed by treatment with HBr and then H2O-Et3N-EtOH gave zwitterion III. III was a mild tranquilizer in mice.

IT 64603-91-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and tranquilizing activity of)

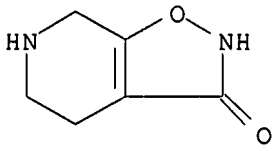
RN 64603-91-4 CAPLUS

CN Isoxazolo[5,4-c]pyridin-3(2H)-one, 4,5,6,7-tetrahydro- (CA INDEX NAME)



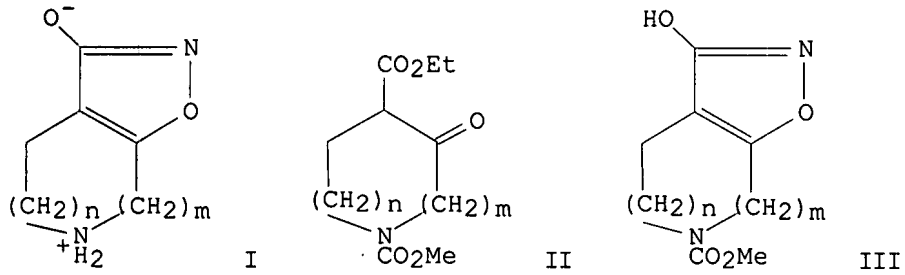
IT 65202-63-3P
RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of)
RN 65202-63-3 CAPLUS
CN Isoxazolo[5,4-c]pyridin-3(2H)-one, 4,5,6,7-tetrahydro-, monohydrobromide (9CI) (CA INDEX NAME)



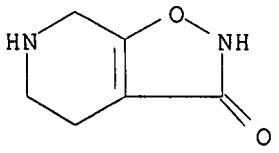
● HBr

L8 ANSWER 8 OF 8 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1978:37672 CAPLUS
DOCUMENT NUMBER: 88:37672
TITLE: Muscimol analogs. II. Synthesis of some bicyclic 3-isoxazolol zwitterions
AUTHOR(S): Krogsgaard-Larsen, Povl
CORPORATE SOURCE: Dep. Chem. BC, R. Dan. Sch. Pharm., Copenhagen, Den.
SOURCE: Acta Chemica Scandinavica, Series B: Organic Chemistry and Biochemistry (1977), B31(7), 584-8
CODEN: ACBOCV; ISSN: 0302-4369
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 88:37672
GI



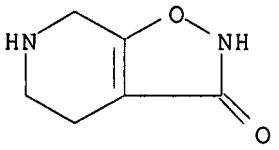
I II III

AB The 3-isoxazolol zwitterions 4,5,6,7-tetrahydroisoxazolo[5,4-c]pyridin-3-ol, (I, n = 1, m = 1), 5,6,7,8-tetrahydro-4H-isoxazolo[5,4-c]azepin-3-ol (I, n = 2, m = 1), and 5,6,7,8-tetrahydro-4H-isoxazolo[4,5-c]azepin-3-ol (I, n = o, m = 3) were prepared The starting materials were the cyclic β-oxoesters II. The ethylene acetals of II were treated with HONH2 followed by deacetalization and cyclization of the intermediate β-oxohydroxamic acid ethylene acetals to give the resp. 3-isoxazolol derivs. III, which were transformed into the zwitterions I. The pKA values of I were determined
IT 65202-63-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction with triethylamine, zwitterions from)
RN 65202-63-3 CAPLUS
CN Isoxazolo[5,4-c]pyridin-3(2H)-one, 4,5,6,7-tetrahydro-, monohydrobromide (9CI) (CA INDEX NAME)



● HBr

IT 64603-91-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 64603-91-4 CAPLUS
CN Isoxazolo[5,4-c]pyridin-3(2H)-one, 4,5,6,7-tetrahydro- (CA INDEX NAME)



=> FIL STNGUIDE

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	51.14	300.80
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-6.24	-16.38

FILE 'STNGUIDE' ENTERED AT 12:49:42 ON 09 MAY 2007
USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT
COPYRIGHT (C) 2007 AMERICAN CHEMICAL SOCIETY, JAPAN SCIENCE
AND TECHNOLOGY CORPORATION, AND FACHINFORMATIONSZENTRUM KARLSRUHE

FILE CONTAINS CURRENT INFORMATION.
LAST RELOADED: May 4, 2007 (20070504/UP).

=> d his

(FILE 'HOME' ENTERED AT 12:37:09 ON 09 MAY 2007)

FILE 'REGISTRY' ENTERED AT 12:38:04 ON 09 MAY 2007
L1 STRUCTURE UPLOADED
L2 36 S L1 FULL

FILE 'CAPLUS' ENTERED AT 12:41:50 ON 09 MAY 2007
L3 13 S L2/PREP FULL
L4 0 S L3 AND NUCLEO?

FILE 'STNGUIDE' ENTERED AT 12:44:01 ON 09 MAY 2007

FILE 'CAPLUS' ENTERED AT 12:48:41 ON 09 MAY 2007
L5 0 S L3 AND LEAV?
L6 13 S L3
L7 0 S L6 AND LEAV?
L8 8 S L6 AND REACT?

FILE 'STNGUIDE' ENTERED AT 12:49:42 ON 09 MAY 2007

=> log y

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.12	300.92

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-16.38

STN INTERNATIONAL LOGOFF AT 12:50:42 ON 09 MAY 2007

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:SSPTANXR1625

PASSWORD:
TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * * * * * * Welcome to STN International * * * * * * * * * *

NEWS 1		Web Page for STN Seminar Schedule - N. America
NEWS 2	JAN 08	CHEMLIST enhanced with New Zealand Inventory of Chemicals
NEWS 3	JAN 16	CA/CAplus Company Name Thesaurus enhanced and reloaded
NEWS 4	JAN 16	IPC version 2007.01 thesaurus available on STN
NEWS 5	JAN 16	WPIDS/WPINDEX/WPIX enhanced with IPC 8 reclassification data
NEWS 6	JAN 22	CA/CAplus updated with revised CAS roles
NEWS 7	JAN 22	CA/CAplus enhanced with patent applications from India
NEWS 8	JAN 29	PHAR reloaded with new search and display fields
NEWS 9	JAN 29	CAS Registry Number crossover limit increased to 300,000 in multiple databases
NEWS 10	FEB 15	PATDPASPC enhanced with Drug Approval numbers
NEWS 11	FEB 15	RUSSIAPAT enhanced with pre-1994 records
NEWS 12	FEB 23	KOREAPAT enhanced with IPC 8 features and functionality
NEWS 13	FEB 26	MEDLINE reloaded with enhancements
NEWS 14	FEB 26	EMBASE enhanced with Clinical Trial Number field
NEWS 15	FEB 26	TOXCENTER enhanced with reloaded MEDLINE
NEWS 16	FEB 26	IFICDB/IFIPAT/IFIUDB reloaded with enhancements
NEWS 17	FEB 26	CAS Registry Number crossover limit increased from 10,000 to 300,000 in multiple databases
NEWS 18	MAR 15	WPIDS/WPIX enhanced with new FRAGHITSTR display format
NEWS 19	MAR 16	CASREACT coverage extended
NEWS 20	MAR 20	MARPAT now updated daily
NEWS 21	MAR 22	LWPI reloaded
NEWS 22	MAR 30	RDISCLOSURE reloaded with enhancements
NEWS 23	APR 02	JICST-EPLUS removed from database clusters and STN
NEWS 24	APR 30	GENBANK reloaded and enhanced with Genome Project ID field
NEWS 25	APR 30	CHEMCATS enhanced with 1.2 million new records
NEWS 26	APR 30	CA/CAplus enhanced with 1870-1889 U.S. patent records
NEWS 27	APR 30	INPADOC replaced by INPADOCDB on STN
NEWS 28	MAY 01	New CAS web site launched
NEWS 29	MAY 08	CA/CAplus Indian patent publication number format defined

NEWS EXPRESS NOVEMBER 10 CURRENT WINDOWS VERSION IS V8.01c, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 25 SEPTEMBER 2006.

NEWS HOURS	STN Operating Hours Plus Help Desk Availability
NEWS LOGIN	Welcome Banner and News Items
NEWS IPC8	For general information regarding STN implementation of IPC 8

Enter NEWS followed by the item number or name to see news on that specific topic.

* * * * * * * * * * * * * * * * STN Columbus * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 08:57:09 ON 09 MAY 2007

=> FILE CASREACT

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'CASREACT' ENTERED AT 08:57:21 ON 09 MAY 2007

FILE CONTENT:1840 - 5 May 2007 VOL 146 ISS 20

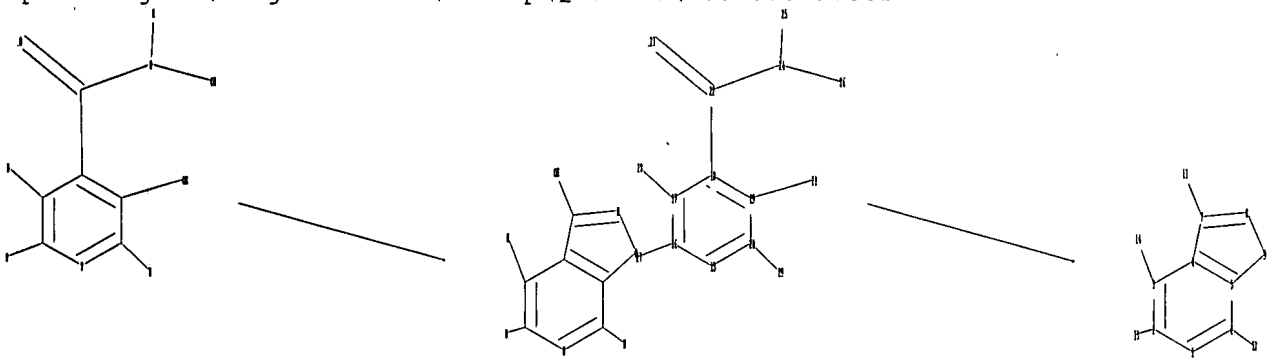
New CAS Information Use Policies, enter HELP USAGETERMS for details.

****
*
* CASREACT now has more than 12 million reactions
*
****

Some CASREACT records are derived from the ZIC/VINITI database (1974-1999) provided by InfoChem, INPI data prior to 1986, and Biotransformations database compiled under the direction of Professor Dr. Klaus Kieslich.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=>
Uploading C:\Program Files\Stnexp\Queries\10570551a.str



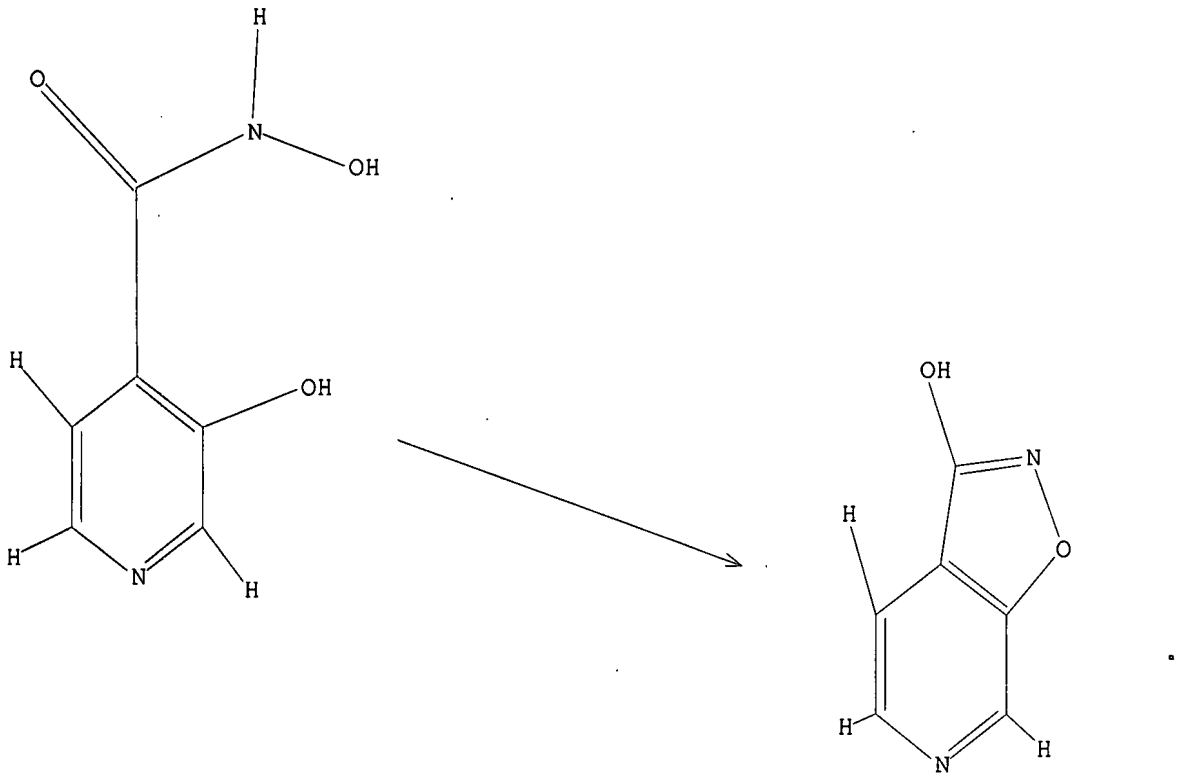
chain nodes :
11 12 13 14 21 22 23 24 25 26 27 28 29
ring nodes :
1 2 3 4 5 6 7 8 9 15 16 17 18 19 20
chain bonds :
2-13 3-14 6-12 7-11 16-27 17-28 18-22 19-21 20-29 22-23 22-24 24-25 24-26

ring bonds :
1-2 1-6 2-3 3-4 4-5 4-7 5-6 5-9 7-8 8-9 15-16 15-20 16-17 17-18 18-19
19-20
exact/norm bonds :
7-8 7-11 19-21 22-23 22-24 24-26
exact bonds :
2-13 3-14 4-7 5-9 6-12 8-9 16-27 17-28 18-22 20-29 24-25
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 15-16 15-20 16-17 17-18 18-19 19-20
isolated ring systems :
containing 1 : 15 :

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 11:CLASS
12:CLASS 13:CLASS 14:CLASS 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom
21:CLASS 22:CLASS 23:CLASS 24:CLASS 25:CLASS 26:CLASS 27:CLASS 28:CLASS
29:CLASS
fragments assigned product role:
containing 1
fragments assigned reactant/reagent role:
containing 15

L1 STRUCTURE UPLOADED

=> d l1
L1 HAS NO ANSWERS
L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l1 full

FULL SEARCH INITIATED 08:57:54 FILE 'CASREACT'
SCREENING COMPLETE - 3 REACTIONS TO VERIFY FROM 2 DOCUMENTS

100.0% DONE 3 VERIFIED 2 HIT RXNS 1 DOCS
SEARCH TIME: 00.00.01

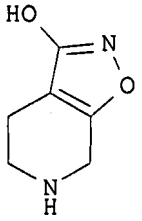
L2 1 SEA SSS FUL L1 (2 REACTIONS)

=> d ibib abs fhit

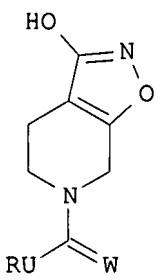
L2 ANSWER 1 OF 1 CASREACT COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 142:316828 CASREACT
TITLE: Method for the manufacture of THIP
INVENTOR(S): Petersen, Hans; Bech Sommer, Michael; Dancer, Robert
PATENT ASSIGNEE(S): H. Lundbeck A/S, Den.
SOURCE: PCT Int. Appl., 34 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005023820	A1	20050317	WO 2004-DK579	20040901
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2004270323	A1	20050317	AU 2004-270323	20040901
CA 2537840	A1	20050317	CA 2004-2537840	20040901
EP 1664060	A1	20060607	EP 2004-762799	20040901
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK, HR				
CN 1845928	A	20061011	CN 2004-80025424	20040901
BR 2004013741	A	20061024	BR 2004-13741	20040901
JP 2007504179	T	20070301	JP 2006-525046	20040901
NO 2006001424	A	20060329	NO 2006-1424	20060329
PRIORITY APPLN. INFO.:			DK 2003-1277	20030905
			US 2003-500422P	20030905
			WO 2004-DK579	20040901

OTHER SOURCE(S): MARPAT 142:316828
GI



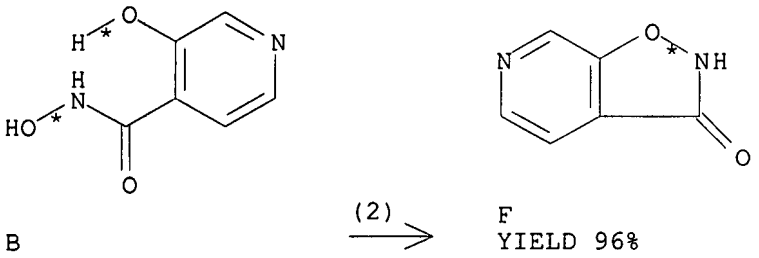
I



II

AB The present invention relates to a new method of preparing gaboxadol (THIP; I), which is useful for treating sleep disorders (no data). In particular a method of preparing THIP comprising reacting a compound II [R = alkyl, cycloalkyl, aryl, etc.; U = N, CR1 (R1 = H, R); W = O, S, NR4 (R4 = H, R)] or a salt thereof with an acid, typically a mineral acid, to obtain THIP as an acid addition salt. The present invention also relates to several intermediates. E.g., a multi-step synthesis of I.HBr, starting from Me 3-hydroxyisonicotinate, was given.

RX(2) OF 15 ...B ===> F...



RX(2) RCT B 89640-77-7
RGT G 530-62-1 Diimidazolyl ketone
PRO F 847996-42-3
SOL 68-12-2 DMF
CON SUBSTAGE(1) room temperature
SUBSTAGE(2) overnight, room temperature
REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d his

(FILE 'HOME' ENTERED AT 08:57:09 ON 09 MAY 2007)

FILE 'CASREACT' ENTERED AT 08:57:21 ON 09 MAY 2007
L1 STRUCTURE UPLOADED
L2 1 S L1 FULL

=> log y

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	118.47	118.68
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-0.73	-0.73

STN INTERNATIONAL LOGOFF AT 08:58:14 ON 09 MAY 2007

claim 1

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:SSPTANXR1625

PASSWORD:
TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * * * * * * Welcome to STN International * * * * * * * * * *

NEWS	1		Web Page for STN Seminar Schedule - N. America
NEWS	2	JAN 08	CHEMLIST enhanced with New Zealand Inventory of Chemicals
NEWS	3	JAN 16	CA/CAplus Company Name Thesaurus enhanced and reloaded
NEWS	4	JAN 16	IPC version 2007.01 thesaurus available on STN
NEWS	5	JAN 16	WPIDS/WPINDEX/WPIX enhanced with IPC 8 reclassification data
NEWS	6	JAN 22	CA/CAplus updated with revised CAS roles
NEWS	7	JAN 22	CA/CAplus enhanced with patent applications from India
NEWS	8	JAN 29	PHAR reloaded with new search and display fields
NEWS	9	JAN 29	CAS Registry Number crossover limit increased to 300,000 in multiple databases
NEWS	10	FEB 15	PATDPASPC enhanced with Drug Approval numbers
NEWS	11	FEB 15	RUSSIAPAT enhanced with pre-1994 records
NEWS	12	FEB 23	KOREAPAT enhanced with IPC 8 features and functionality
NEWS	13	FEB 26	MEDLINE reloaded with enhancements
NEWS	14	FEB 26	EMBASE enhanced with Clinical Trial Number field
NEWS	15	FEB 26	TOXCENTER enhanced with reloaded MEDLINE
NEWS	16	FEB 26	IFICDB/IFIPAT/IFIUDB reloaded with enhancements
NEWS	17	FEB 26	CAS Registry Number crossover limit increased from 10,000 to 300,000 in multiple databases
NEWS	18	MAR 15	WPIDS/WPIX enhanced with new FRAGHITSTR display format
NEWS	19	MAR 16	CASREACT coverage extended
NEWS	20	MAR 20	MARPAT now updated daily
NEWS	21	MAR 22	LWPI reloaded
NEWS	22	MAR 30	RDISCLOSURE reloaded with enhancements
NEWS	23	APR 02	JICST-EPLUS removed from database clusters and STN
NEWS	24	APR 30	GENBANK reloaded and enhanced with Genome Project ID field
NEWS	25	APR 30	CHEMCATS enhanced with 1.2 million new records
NEWS	26	APR 30	CA/CAplus enhanced with 1870-1889 U.S. patent records
NEWS	27	APR 30	INPADOC replaced by INPADOCDB on STN
NEWS	28	MAY 01	New CAS web site launched
NEWS	29	MAY 08	CA/CAplus Indian patent publication number format defined

NEWS EXPRESS NOVEMBER 10 CURRENT WINDOWS VERSION IS V8.01c, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 25 SEPTEMBER 2006.

NEWS HOURS	STN Operating Hours Plus Help Desk Availability
NEWS LOGIN	Welcome Banner and News Items
NEWS IPC8	For general information regarding STN implementation of IPC 8

Enter NEWS followed by the item number or name to see news on that specific topic.

* * * * * * * * * * * * * * * * STN Columbus * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 08:49:51 ON 09 MAY 2007

=> file casreact
COST IN U.S. DOLLARS

	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'CASREACT' ENTERED AT 08:50:30 ON 09 MAY 2007

FILE CONTENT:1840 - 5 May 2007 VOL 146 ISS 20

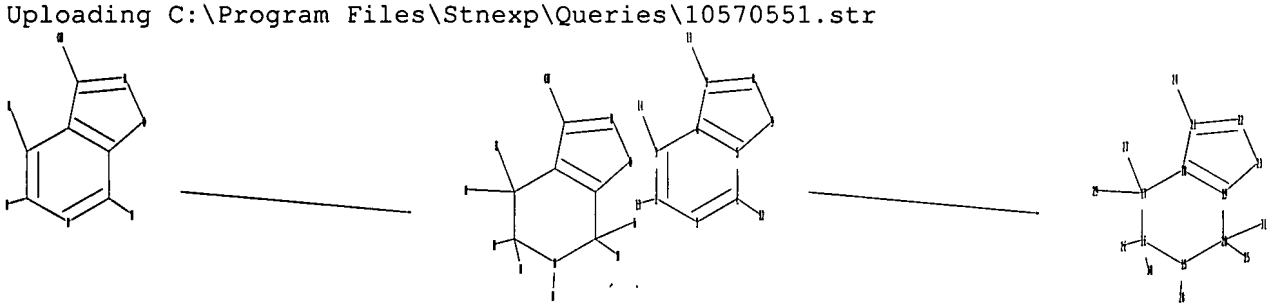
New CAS Information Use Policies, enter HELP USAGETERMS for details.

****
*
* CASREACT now has more than 12 million reactions
*
****

Some CASREACT records are derived from the ZIC/VINITI database (1974-1999) provided by InfoChem, INPI data prior to 1986, and Biotransformations database compiled under the direction of Professor Dr. Klaus Kieslich.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=>
Uploading C:\Program Files\Stnexp\Queries\10570551.str



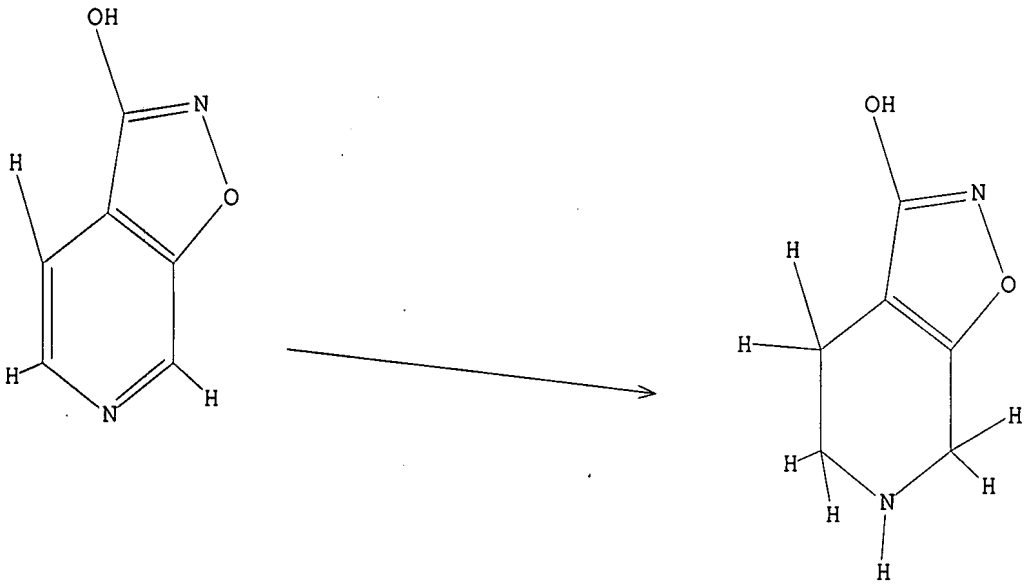
chain nodes :
11 12 13 14 24 25 26 27 28 29 30 31
ring nodes :
1 2 3 4 5 6 7 8 9 15 16 17 18 19 20 21 22 23
chain bonds :
2-13 3-14 6-12 7-11 15-28 16-26 16-30 17-27 17-29 20-25 20-31 21-24
ring bonds :
1-2 1-6 2-3 3-4 4-5 4-7 5-6 5-9 7-8 8-9 15-16 15-20 16-17 17-18 18-19 18-21 19-20 19-23 21-22 22-23
exact/norm bonds :
7-8 7-11 15-16 15-20 16-17 17-18 18-19 18-21 19-20 19-23 21-22 21-24 22-23

exact bonds :
2-13 3-14 4-7 5-9 6-12 8-9 15-28 16-26 16-30 17-27 17-29 20-25 20-31
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6
isolated ring systems :
containing 1 :

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 11:CLASS
12:CLASS 13:CLASS 14:CLASS 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom
21:Atom 22:Atom 23:Atom 24:CLASS 25:CLASS 26:CLASS 27:CLASS 28:CLASS
29:CLASS 30:CLASS 31:CLASS
fragments assigned product role:
containing 15
fragments assigned reactant/reagent role:
containing 1

L1 STRUCTURE UPLOADED

=> d l1
L1 HAS NO ANSWERS
L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l1 full
FULL SEARCH INITIATED 08:51:09 FILE 'CASREACT'
SCREENING COMPLETE - 3 REACTIONS TO VERIFY FROM 1 DOCUMENTS

100.0% DONE 3 VERIFIED 2 HIT RXNS 1 DOCS
SEARCH TIME: 00.00.01

L2 1 SEA SSS FUL L1 (2 REACTIONS)

=> d ibib abs fhitstr tot
'FHITSTR' IS NOT A VALID FORMAT FOR FILE 'CASREACT'

The following are valid formats:

ABS -------- GI and AB
ALL -------- BIB, AB, IND, RE, Single-step Reactions
APPS ------- AI, PRAI
BIB -------- AN, plus Bibliographic Data
CAN -------- List of CA abstract numbers without answer numbers
CBIB ------- AN, plus Compressed Bibliographic Data
DALL ------- ALL, delimited (end of each field identified)
IABS ------- ABS, indented with text labels
IALL ------- ALL, indented with text labels
IBIB ------- BIB, indented with text labels
IND -------- Indexing data
IPC -------- International Patent Classifications
ISTD ------- STD, indented with text labels
OBIB -------- AN, plus Bibliographic Data (original)
OIBIB ------- OBIB, indented with text labels

SBIB -------- BIB, no citations
SIBIB ------- IBIB, no citations

MAX -------- Same as ALL
PATS ------- PI, SO
SCAN ------- TI and FCRD (random display, no answer number. SCAN must be entered on the same line as DISPLAY, e.g., D SCAN.)
SSRX ------- Single-Step Reactions (Map, Diagram, and Summary for all single-step reactions)
STD -------- BIB, IPC, and NCL

CRD -------- Compact Display of All Hit Reactions
CRDREF ----- Compact Reaction Display and SO, PY for Reference
FHIT ------- Reaction Map, Diagram, and Summary for first hit reaction
FHITCBIB --- FHIT, AN plus CBIB
FCRD ------- First hit in Compact Reaction Display (CRD) format
FCRDREF ---- First hit in Compact Reaction Display (CRD) format with CA reference information (SO, PY). (Default)
FPATH ------ PATH, plus Reaction Summary for the "long path"
FSPATH ----- SPATH, plus Reaction Summary for the "short path"
HIT -------- Reaction Map, Reaction Diagram, and Reaction Summary for all hit reactions and fields containing hit terms
OCC -------- All hit fields and the number of occurrences of the hit terms in each field. Includes total number of HIT, PATH, SPATH reactions. Labels reactions that have incomplete verifications.
PATH ------- Reaction Map and Reaction Diagram for the "long path". Displays all hit reactions, except those whose steps are totally included within another hit reaction which is displayed
RX --------- Hit Reactions (Map, Diagram, Summary for all hit reactions)
RXG -------- Hit Reaction Graphics (Map and Diagram for all hit reactions)
RXL -------- Hit Reaction Long (Map, Diagram, Summary for all hit reactions)
RXS -------- Hit Reaction Summariers (Map and Summary for all hit reactions)
SPATH ------ Reaction Map and Reaction Diagram for the "short path". Displays all single step reactions which contain a hit substance. Also displays those multistep reactions that have a hit substance in both the first and last steps of the reaction, except for those hit reactions whose steps are totally included within another hit reaction which is displayed

To display a particular field or fields, enter the display field codes. For a list of the display field codes, enter HELP DFIELDS

at an arrow prompt (=>). Examples of combinations include: D TI; D BIB RX; D TI, AU, FCRD. The information is displayed in the same order as the specification. All of the formats, except CRD, CRDREF, FHIT, PATH, FPATH, SPATH, FSPATH, FCRD, FCRDREF, HIT, RX, RXG, RXS, SCAN, and OCC, may be used with the DISPLAY command to display the record for a specified Accession Number.

ENTER DISPLAY FORMAT (FCRDREF):cbib

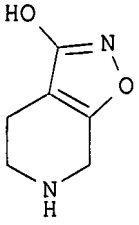
L2 ANSWER 1 OF 1 CASREACT COPYRIGHT 2007 ACS on STN
142:316828 Method for the manufacture of THIP. Petersen, Hans; Bech Sommer, Michael; Dancer, Robert (H. Lundbeck A/S, Den.). PCT Int. Appl. WO 2005023820 A1 20050317, 34 pp. DESIGNATED STATES: W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG, TR. (English). CODEN: PIXXD2. APPLICATION: WO 2004-DK579 20040901. PRIORITY: DK 2003-1277 20030905; US 2003-2003/PV500422 20030905.

=> d ibib abs fhit

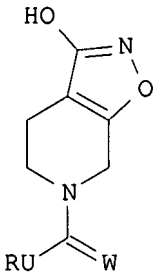
L2 ANSWER 1 OF 1 CASREACT COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 142:316828 CASREACT
TITLE: Method for the manufacture of THIP
INVENTOR(S): Petersen, Hans; Bech Sommer, Michael; Dancer, Robert
PATENT ASSIGNEE(S): H. Lundbeck A/S, Den.
SOURCE: PCT Int. Appl., 34 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005023820	A1	20050317	WO 2004-DK579	20040901
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2004270323	A1	20050317	AU 2004-270323	20040901
CA 2537840	A1	20050317	CA 2004-2537840	20040901
EP 1664060	A1	20060607	EP 2004-762799	20040901
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK, HR				
CN 1845928	A	20061011	CN 2004-80025424	20040901
BR 2004013741	A	20061024	BR 2004-13741	20040901
JP 2007504179	T	20070301	JP 2006-525046	20040901
NO 2006001424	A	20060329	NO 2006-1424	20060329
PRIORITY APPLN. INFO.:			DK 2003-1277	20030905
			US 2003-500422P	20030905

OTHER SOURCE(S): MARPAT 142:316828
GI



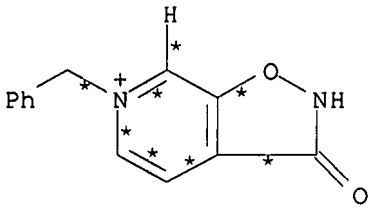
I



II

AB The present invention relates to a new method of preparing gaboxadol (THIP; I), which is useful for treating sleep disorders (no data). In particular a method of preparing THIP comprising reacting a compound II [R = alkyl, cycloalkyl, aryl, etc.; U = N, CR1 (R1 = H, R); W = O, S, NR4 (R4 = H, R)] or a salt thereof with an acid, typically a mineral acid, to obtain THIP as an acid addition salt. The present invention also relates to several intermediates. E.g., a multi-step synthesis of I.HBr, starting from Me 3-hydroxyisonicotinate, was given.

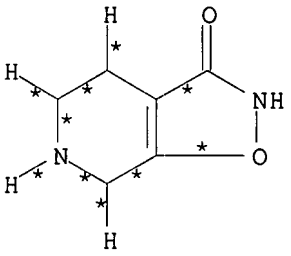
RX(9) OF 15 COMPOSED OF RX(4), RX(5)
RX(9) J ===> O



● Br^-

J

2
STEPS



● HBr

O
YIELD 68%

RX(4) RCT J 847996-43-4
RGT M 16940-66-2 NaBH4
PRO L 847996-44-5
SOL 7732-18-5 Water, 64-17-5 EtOH
CON SUBSTAGE(1) <35 deg C
SUBSTAGE(2) 24 hours
NTE caution reagent foams on addition

RX(5) RCT L 847996-44-5

STAGE(1)
RGT P 7087-68-5 EtN(Pr-i)2, Q 79-22-1 ClCO2Me

```
               SOL  141-78-6 AcOEt
               CON  SUBSTAGE(1) room temperature
                    SUBSTAGE(2) 48 hours, room temperature
                    SUBSTAGE(3) room temperature -> 0 deg C

            STAGE(2)
               RGT  R 7664-41-7 NH3
               SOL  7732-18-5 Water
               CON  SUBSTAGE(2) 15 minutes

            STAGE(3)
               RGT  S 10035-10-6 HBr
               SOL  64-19-7 AcOH
               CON  SUBSTAGE(2) 6 hours, 40 deg C

          PRO  O 65202-63-3
REFERENCE COUNT:          3     THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS
                                RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT


=> d his

     (FILE 'HOME' ENTERED AT 08:49:51 ON 09 MAY 2007)

     FILE 'CASREACT' ENTERED AT 08:50:30 ON 09 MAY 2007
L1              STRUCTURE UPLOADED
L2            1 S L1 FULL

=> log y
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                       ENTRY    SESSION
FULL ESTIMATED COST                                   120.95     121.16

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)          SINCE FILE      TOTAL
                                                       ENTRY    SESSION
CA SUBSCRIBER PRICE                                    -0.73      -0.73

STN INTERNATIONAL LOGOFF AT 08:53:01 ON 09 MAY 2007
```